

Crystal structures
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Auguste Bravais; 23 August 1811, Annonay, Ardèche – 30 March 1863, Le Chesnay, France) was a French physicist, well known for his work in crystallography (the Bravais lattices, and the Bravais laws). Bravais also studied magnetism, the northern lights, meteorology, geobotany or phyllotaxis, astronomy, and hydrography.

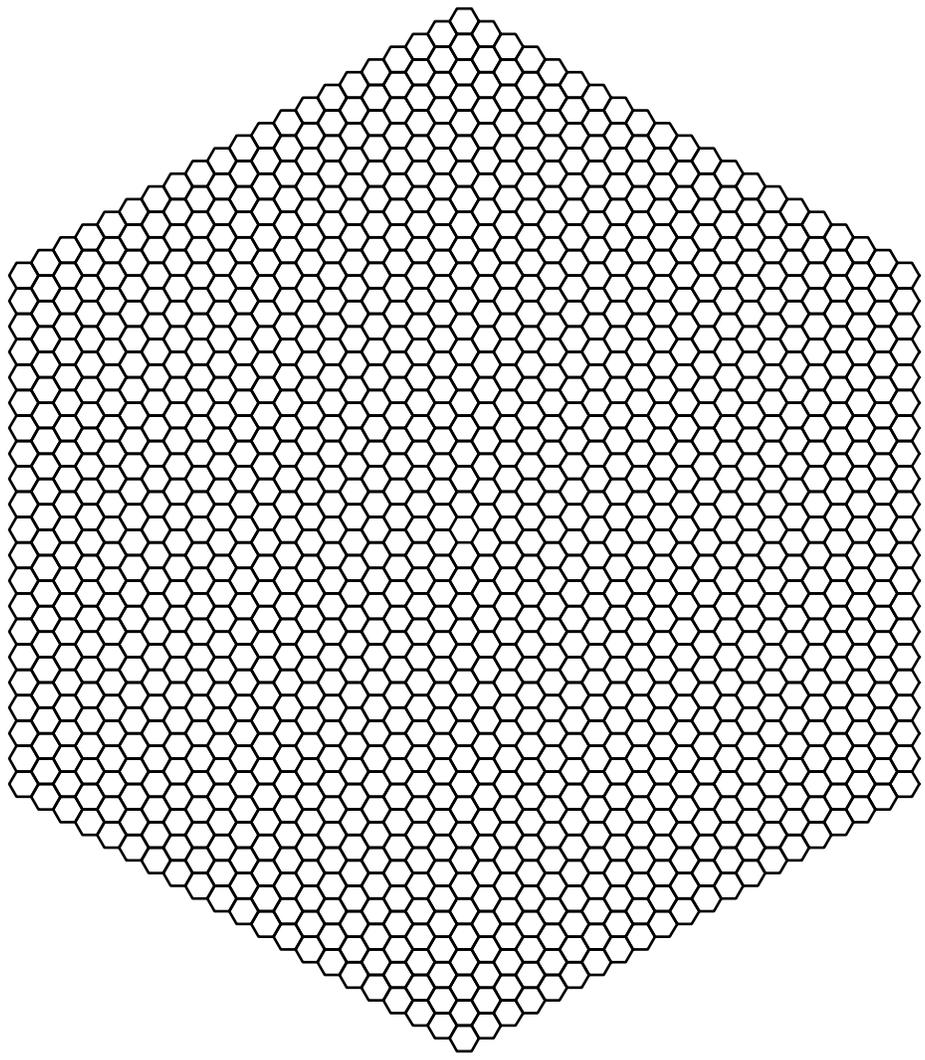


http://en.wikipedia.org/wiki/Auguste_Bravais

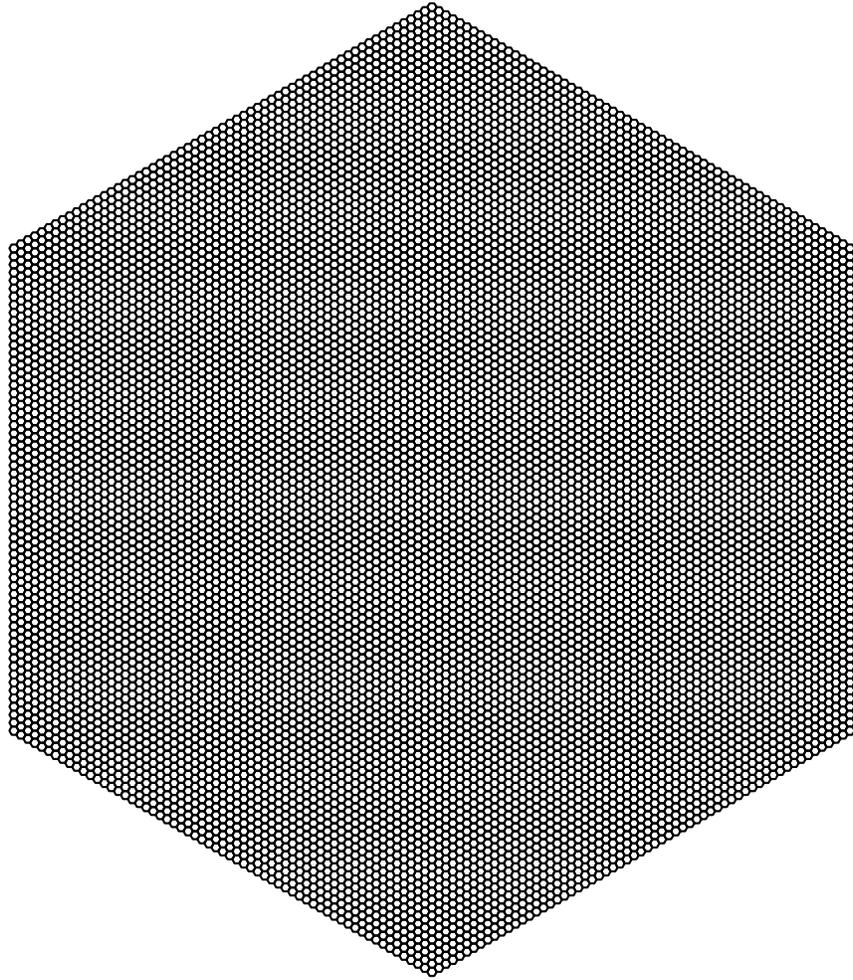
Dan Shechtman (Hebrew: דן שכטמן) (born January 24, 1941 in Tel Aviv) is the *Philip Tobias Professor of Materials Science* at the Technion – Israel Institute of Technology, an Associate of the US Department of Energy's Ames Laboratory, and Professor of Materials Science at Iowa State University. On April 8, 1982, while on sabbatical at the U.S. National Bureau of Standards in Washington, D.C., Shechtman discovered the icosahedral phase, which opened the new field of quasiperiodic crystals. He was awarded the 2011 Nobel Prize in Chemistry for "the discovery of quasicrystals".



http://en.wikipedia.org/wiki/Dan_Shechtman



Graphene lattice



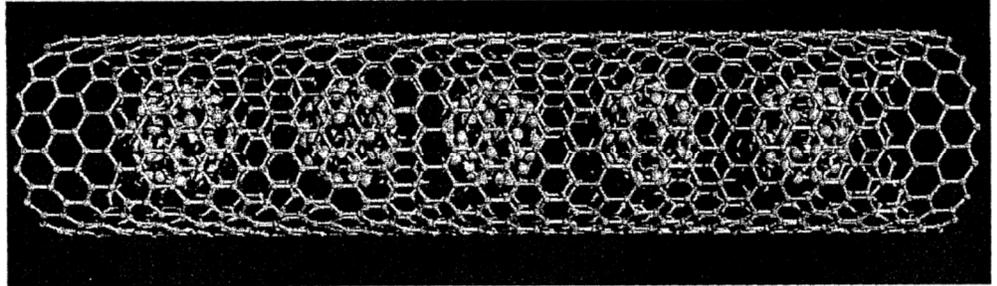


Figure 12.10 Typical single-wall carbon nanotube with C_{60} molecules inside (called peapod) (Hirahara et al., 2000).

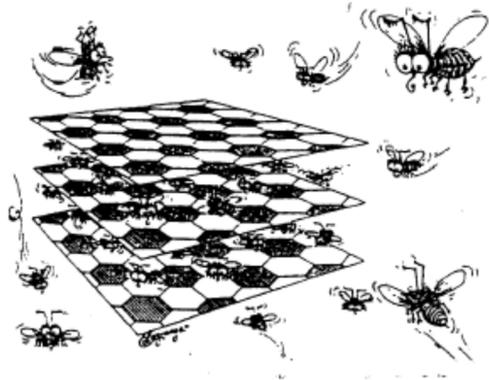


Fig. Formulation of graphite intercalation compounds.

((Note)) Avogadro number, cm, and lattice constant

A volume of typical sample is $V = 1 \text{ cm}^3$. Suppose that the system has a simple cubic lattice with a lattice constant a . Each unit cell has a volume of a^3 . The system consists of the Avogadro number of unit cells. So we get

$$V = N_A a^3 = L^3$$

where L is side of the typical sample. L is evaluated as

$$L = N_A^{1/3} a$$

Noting that

$$N_A^{1/3} = 8.44469 \times 10^7 = 0.844469 \times 10^8.$$

we have

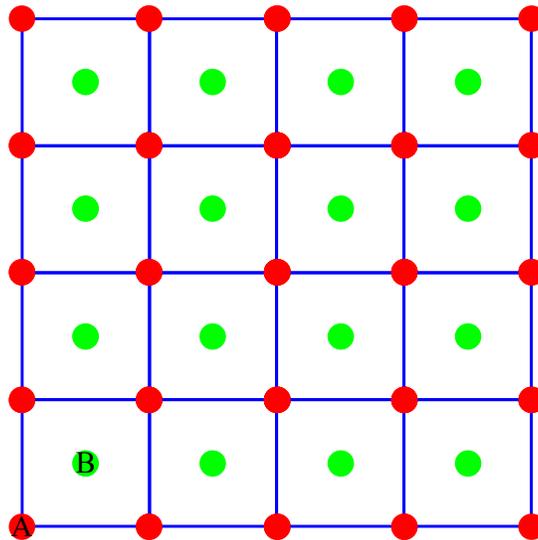
$$L(\text{cm}) = 0.844469 a (\text{\AA})$$

In other words, when $L = 1 \text{ cm}$, a is evaluated as

$$a = 1.18418 \text{\AA}.$$

1. Introduction

An ideal crystal is constructed by the infinite repetition of identical structural units in space.



The structures of all crystals can be described in terms of a **lattice** (A), with a group of atoms (B) attached to every lattice point (**basis**).

2. Lattice point

There are many choices of lattice points. We show two examples.

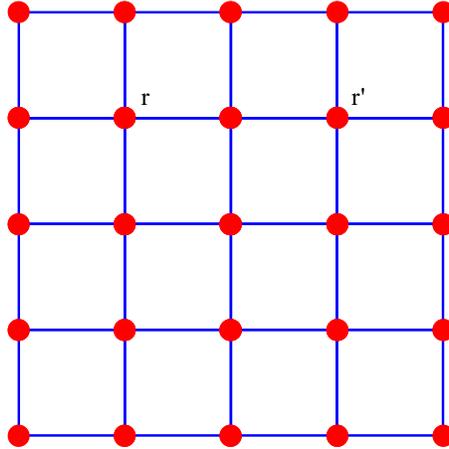


Fig. 2D square lattice. r and r' are lattice points.

or

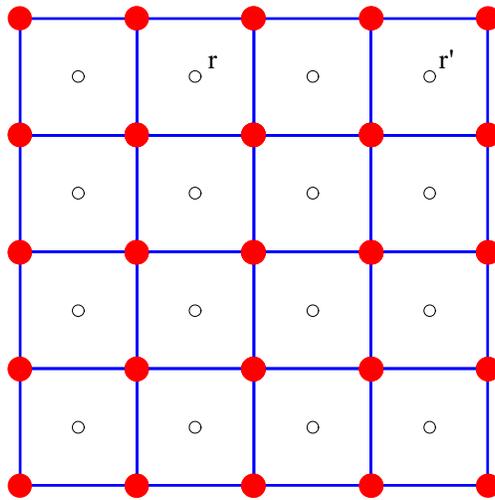


Fig. 2D square lattice. Another choice of lattice points. r and r' are lattice points.

The atomic arrangement in the crystal looks exactly the same to an observer at r' as to an observer at r .

2. Basis

The group of atoms is called the **basis**; when repeated in space it forms the crystal structure. A basis of atoms is attached to every lattice point.

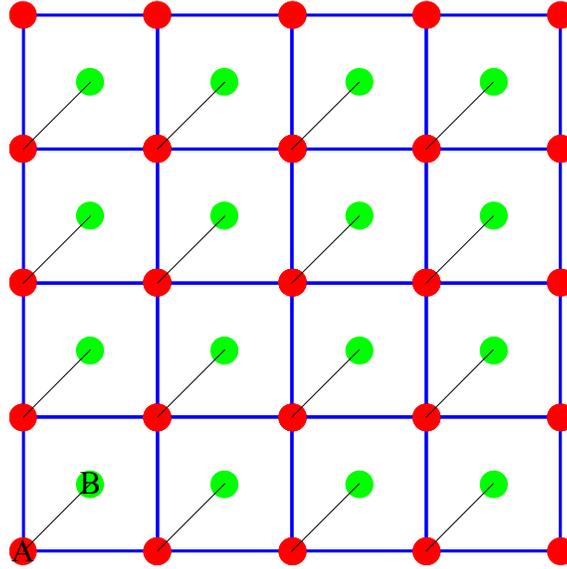


Fig. Crystal structure with lattice point (A) and basis (A-B).

The crystal structures are formed when a basis of atoms is attached identically to every lattice point.

Lattice + basis = crystal structure

3. The three dimensional (3D) structures

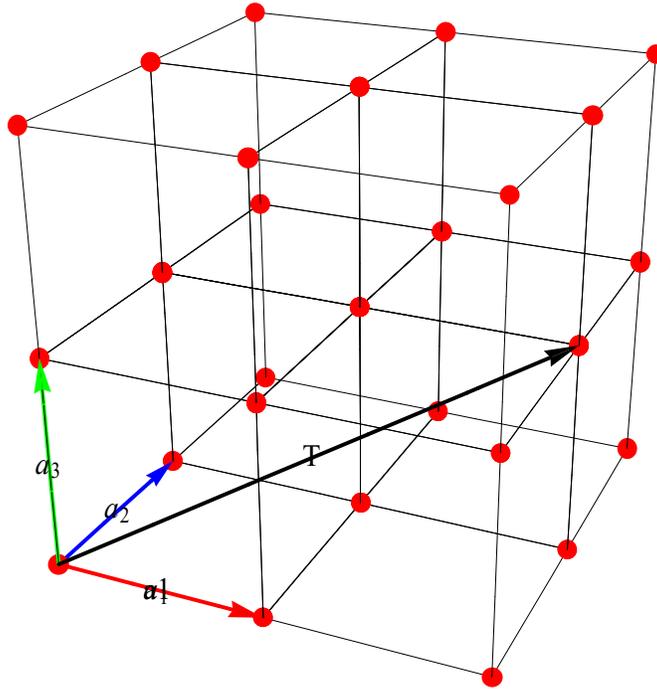


Fig. 3D lattice. \mathbf{a}_1 , \mathbf{a}_2 , and \mathbf{a}_3 are primitive lattice vectors. Lattice points (red circles). \mathbf{T} is the translation vector; $\mathbf{T} = 2\mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3$.

The lattice is defined by three primitive translation vectors, \mathbf{a}_1 , \mathbf{a}_2 , and \mathbf{a}_3 ,

$$\mathbf{T} = u_1\mathbf{a}_1 + u_2\mathbf{a}_2 + u_3\mathbf{a}_3, \quad (\text{lattice point})$$

where u_1, u_2, u_3 are integers. The lattice is defined by three primitive translation vectors, \mathbf{a}_1 , \mathbf{a}_2 , and \mathbf{a}_3 . A lattice translation operation is defined as the displacement of a crystal by a crystal translation vector.

The number of atoms in the basis may be one or it may be more than one.

$$\mathbf{r}_j = x_j\mathbf{a}_1 + y_j\mathbf{a}_2 + z_j\mathbf{a}_3 \quad (\text{basis})$$

where $0 \leq x_j, y_j, z_j < 1$.

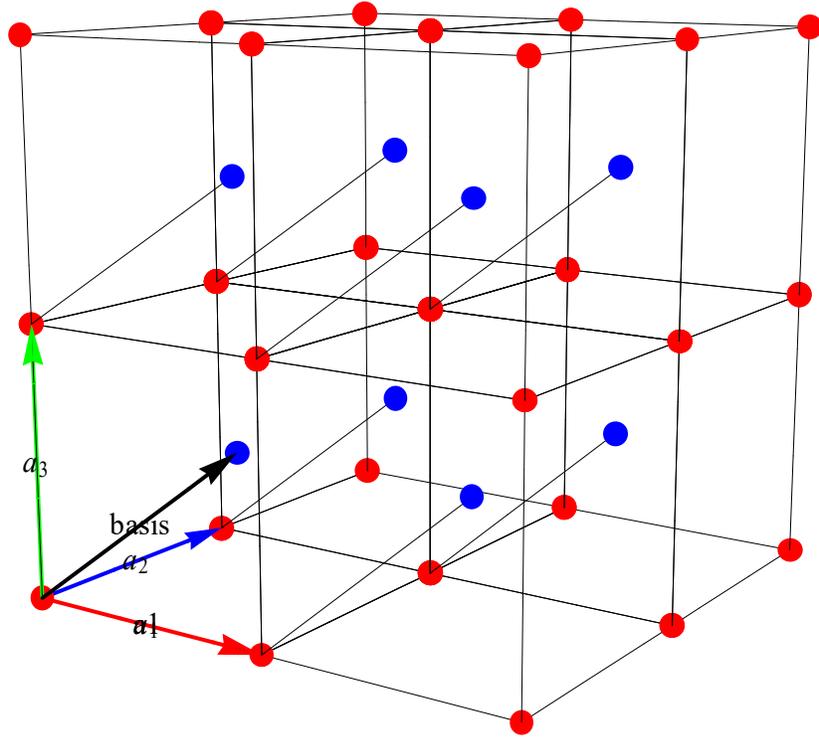
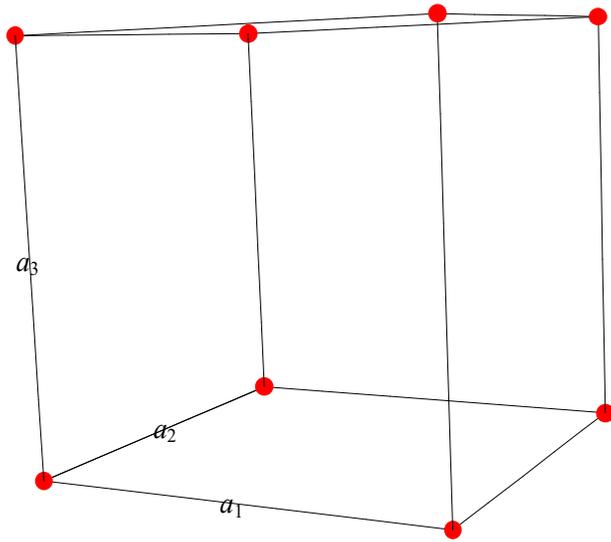


Fig. 3D lattice. Lattice point + basis.

4. Primitive lattice cell

The parallel-piped defined by primitive axes a_1 , a_2 , a_3 is called a primitive cell. A primitive cell is a minimum-volume cell.



There is always one lattice point per primitive cell (definition). If the primitive cell is a parallel-piped with lattice points at each of eight corners, each lattice point is shared among eight corners, so that the total number of lattice points in the cell is one,

$$8 \times \frac{1}{8} = 1.$$

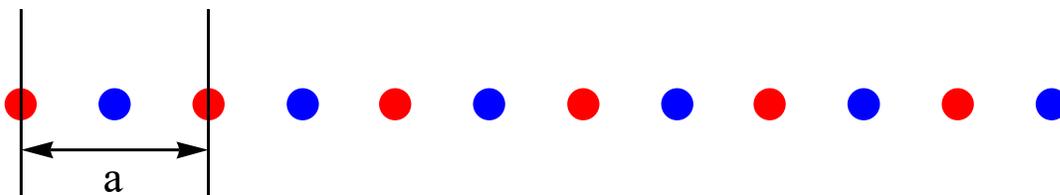
The volume of a parallel-piped with primitive axes \mathbf{a}_1 , \mathbf{a}_2 , \mathbf{a}_3 is

$$V_c = |\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)| = |\mathbf{a}_2 \cdot (\mathbf{a}_3 \times \mathbf{a}_1)| = |\mathbf{a}_3 \cdot (\mathbf{a}_1 \times \mathbf{a}_2)|.$$

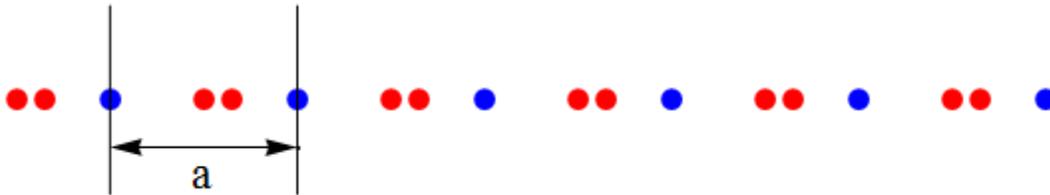
The basis associated with a primitive lattice cell is called a primitive basis.

5. Example

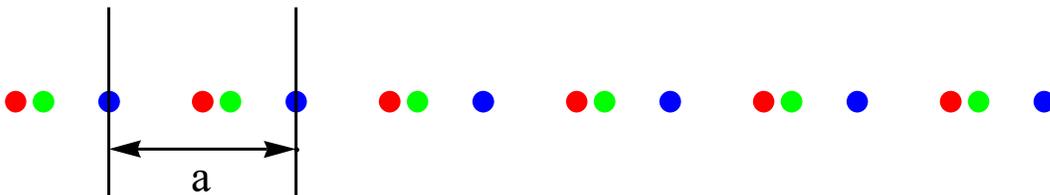
(1) 1D system (linear chain)



The primitive cell: a . Basis: the position of the blue point is denoted by $a/2$, as well as the red atom at the origin.



The primitive cell: a . Basis: red atoms at u_1a and u_2a , as well as blue atom at the origin. The primitive basis consists of two identical atoms, one at u_1a and the other at u_2a .



The primitive cell: a . Basis: red atoms at u_1a , green atom at u_2a , as well as blue atom at the origin.

- (2) 2D systems
- (a) Graphene

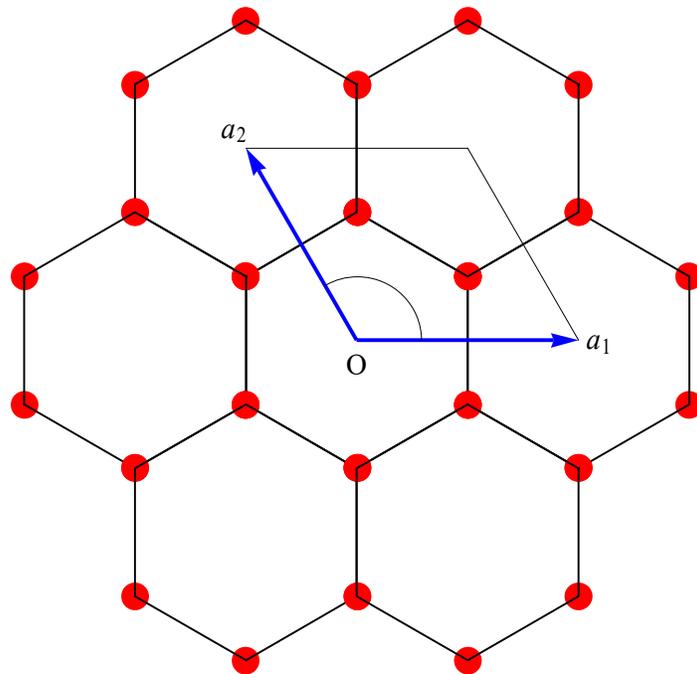
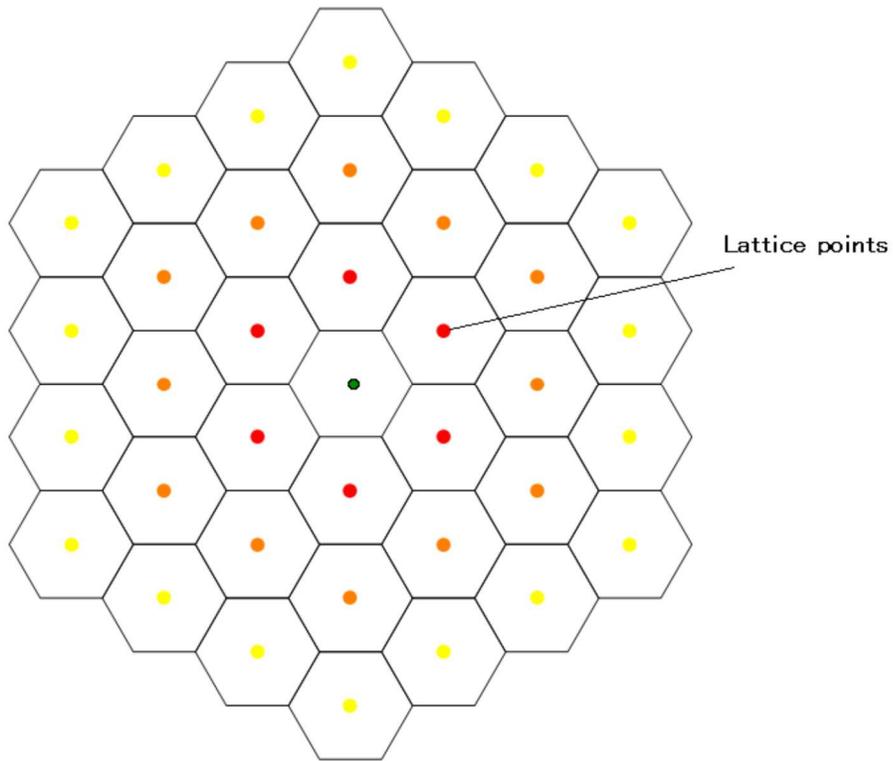
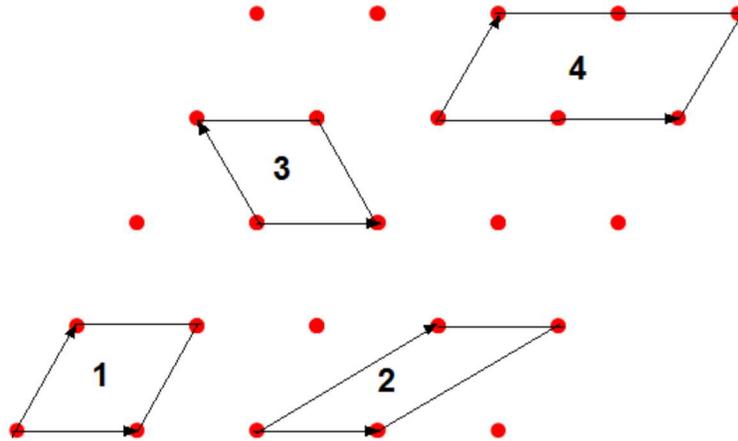


Fig. Graphite. Primitive unit cell. Basis (two identical C atoms). hexagonal lattice.

(b) Example

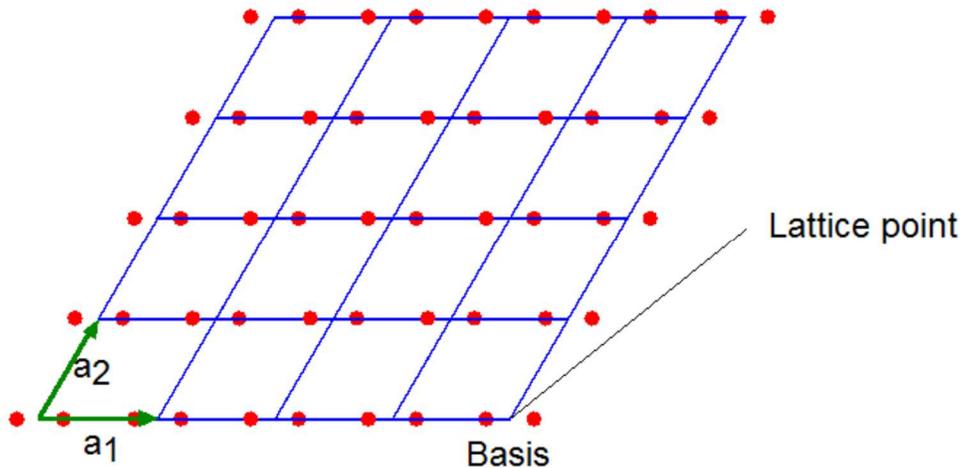


1, 2, 3: Primitive cell (there is one lattice point)
 4: Conventional cell (there are 2 lattice points)

((Definition)) Conventional cell

If there are more than one lattice point in the cell, the cell is called the conventional cell. Later we discuss the conventional cell for the 3D systems.

(c) Example



a_1 and a_2 are primitive translation vector.
 a_1 and a_2 are primitive axes.

(d) Example

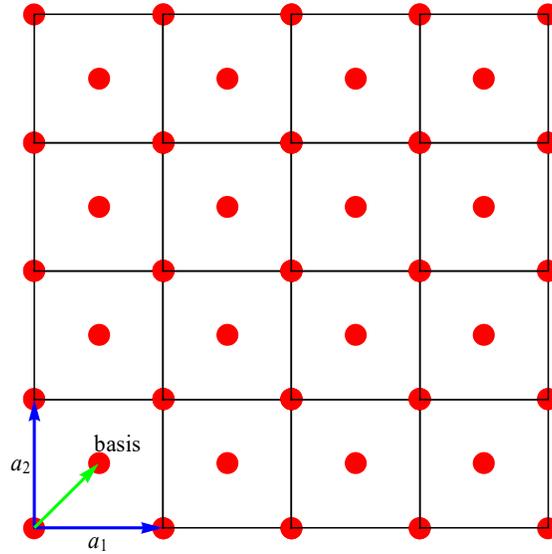


Fig. Conventional cell ($a_1 \times a_2$). There are two lattice points in this cell.

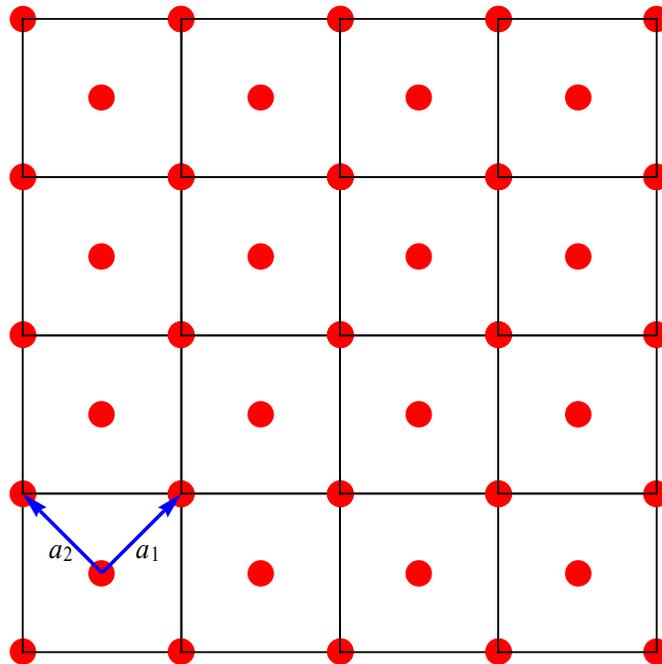


Fig. Primitive cell ($a_1 \times a_2$). There is one lattice point per this cell. a_1 and a_2 are the primitive translation vectors

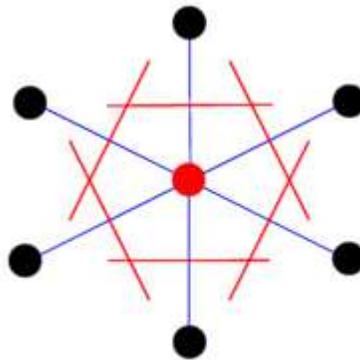
((Summary))

1. Crystal has a primitive cell.
2. Lattice point is defined in association with primitive cell.
3. There is one lattice point per primitive cell.
4. Conventional cell (or nonprimitive cell) contains more than one lattice points.

6. Wigner-Seitz cell

A Wigner–Seitz cell is an example of another kind of primitive cell which has only one lattice point. This Wigner-Seitz cell can be constructed as follows.

- (i) Draw lines to connect a given lattice point to all nearby lattice points.
- (ii) At the midpoint and normal to these lines, draw new lines or planes.



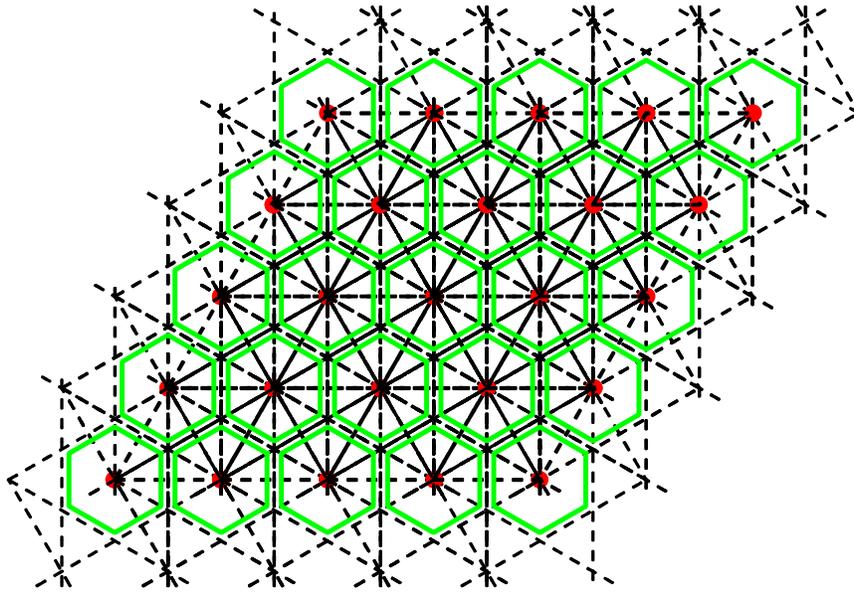


Fig. Typical example of the Wigner-Seitz cell (one of the primitive cells). The dotted line denotes the perpendicular bisector.

((Example-I))

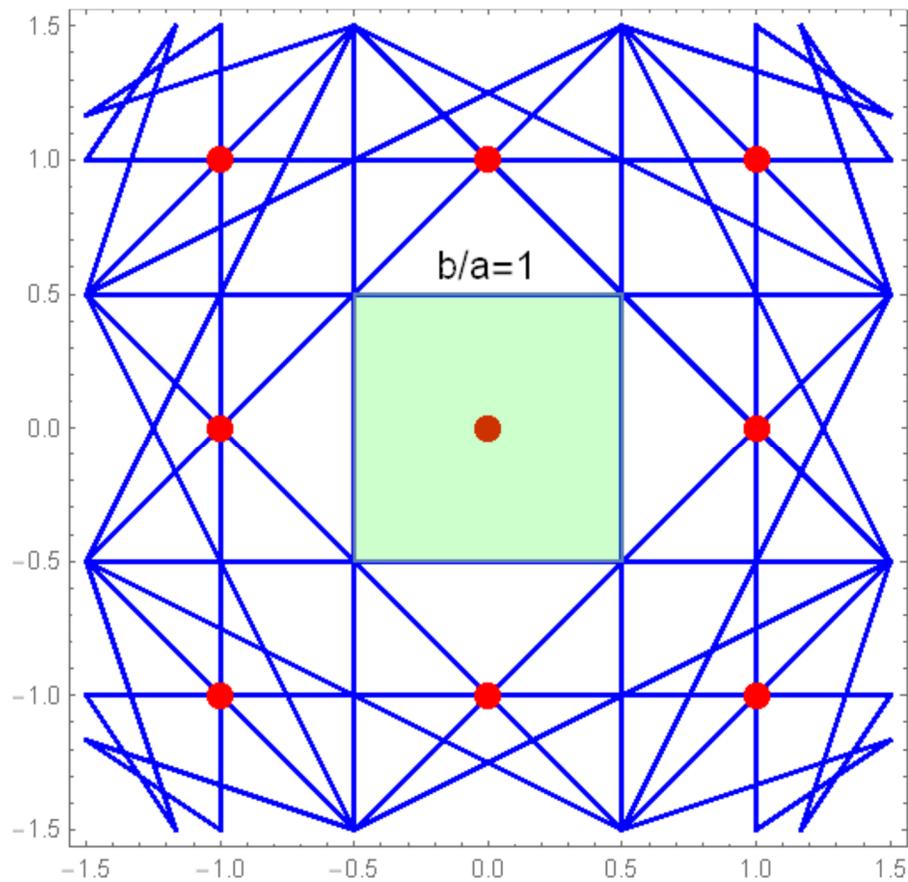
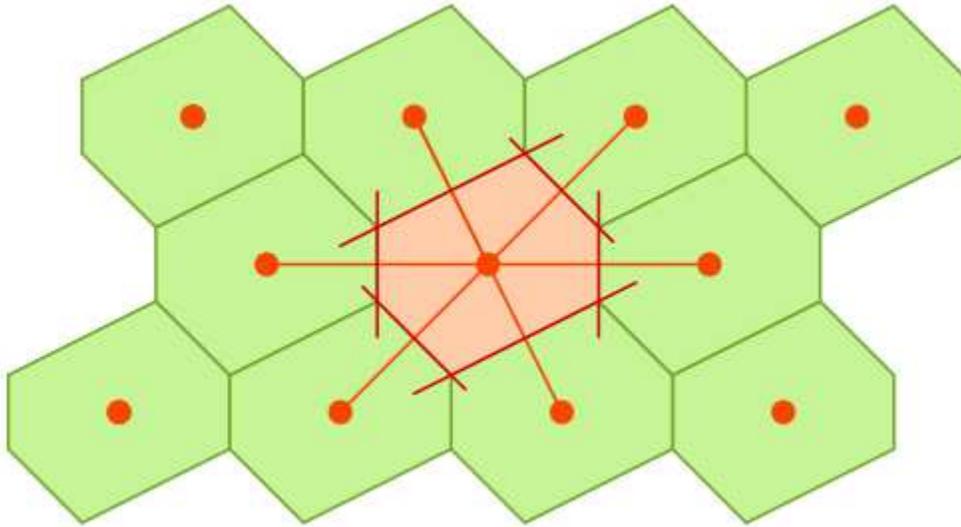


Fig. Example of 2D-construction of a Wigner-Seitz cell (shaded by Green) for the square lattice. Note that such construction in the real space is similar to that of the Brillouin zone in the reciprocal lattice (see the construction of Brillouin zone in later chapter).

((Example-II))



<https://www.physics-in-a-nutshell.com/article/5/unit-cell-primitive-cell-and-wigner-seitz-cell#wigner-seitz-cell>

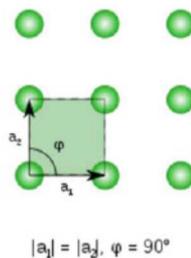
Fig. Example of 2D-construction of a Wigner-Seitz cell: One chooses any lattice point and draws connecting lines to its closest neighbors. In a second step one constructs the perpendicular bisectors of the connecting lines. The enclosed area is the Wigner-Seitz cell. It forms a primitive unit cell. There is only one lattice point in this unit cell.

7. Two dimensional lattice type

Bravais lattice (common phrase for a distinct lattice type)

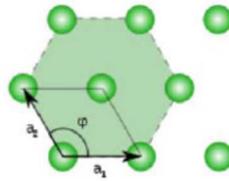
(a) Square lattice (4mm)

The square lattice is invariant under rotation of $2\pi/4$ about any lattice point (point operation 4)



(b) **Hexagonal lattice (6mm)**

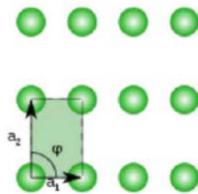
The hexagonal lattice is invariant under rotation of $2\pi/6$ about lattice point (point rotation 3 and 6).



$$|a_1| = |a_2|, \varphi = 120^\circ$$

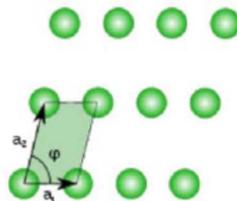
(c) **Rectangular lattice (2mm)**

The rectangular lattice has mirror-symmetry line.



(d) **Oblique lattice**

The oblique lattice is invariant only under rotation of π and 2π about any lattice point.

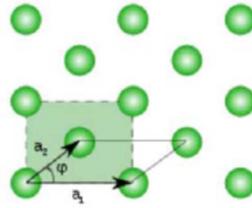


$$|a_1| \neq |a_2|, \varphi \neq 90^\circ$$

(e) **Centered rectangular lattice (2mm)**

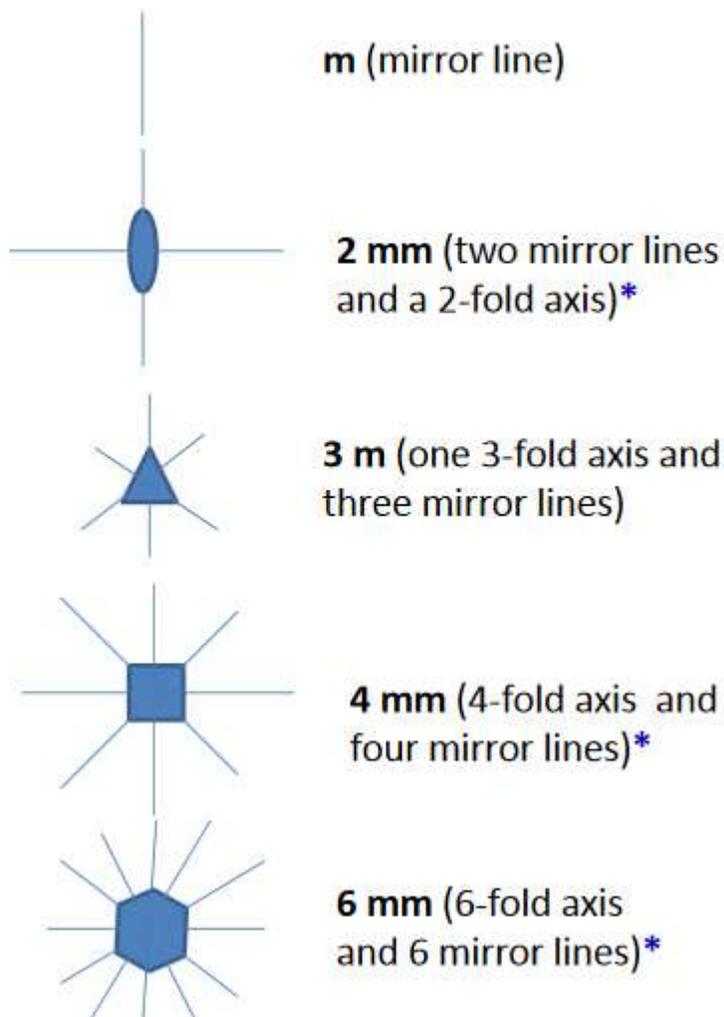
Conventional lattice: there are two lattice points per the cell.

Primitive lattice: there is one lattice point. ($a_1 \times a_2$)



$$|a_1| \neq |a_2|, \phi \neq 90^\circ$$

((Note)) **Crystallographic plane point groups**



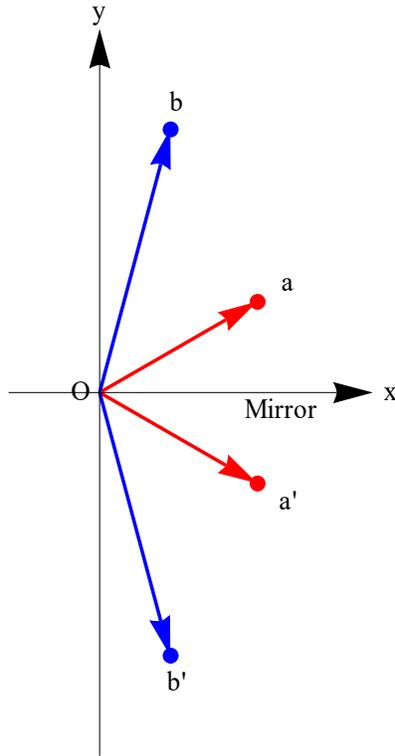
*: Second “m” in the symbol refers to the second type of mirror line. In other words, there are two types of mirror lines.

8. Mirror reflection

We note that the square and hexagonal lattices possess in addition two sets of mirror planes, but oblique lattices in general do not have reflection symmetry. When they do, two additional lattice types result.

Suppose that mirror reflection m is present for the system. The primitive translation vectors are given by

$$\mathbf{a} = a_x \mathbf{e}_x + a_y \mathbf{e}_y, \quad \mathbf{b} = b_x \mathbf{e}_x + b_y \mathbf{e}_y$$



If the lattice is invariant under the reflection (along the x axis), \mathbf{a}' and \mathbf{b}' must be lattice vectors,

$$\mathbf{a}' = a_x \mathbf{e}_x - a_y \mathbf{e}_y, \quad \mathbf{b}' = b_x \mathbf{e}_x - b_y \mathbf{e}_y$$

$\mathbf{a} + \mathbf{a}'$, $\mathbf{a} - \mathbf{a}'$, $\mathbf{b} + \mathbf{b}'$, $\mathbf{b} - \mathbf{b}'$ must be also lattice vectors.

$$\mathbf{a} + \mathbf{a}' = 2a_x \mathbf{e}_x, \quad \mathbf{b} + \mathbf{b}' = 2b_x \mathbf{e}_x$$

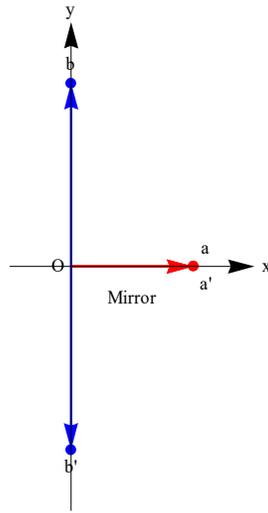
$$\mathbf{a} - \mathbf{a}' = 2a_y \mathbf{e}_y, \quad \mathbf{b} - \mathbf{b}' = 2b_y \mathbf{e}_y$$

Here we choose the two cases

(1) $a_y = 0$, and $b_x = 0$ (rectangular lattice),

$$\mathbf{a} = a_x \mathbf{e}_x, \quad \mathbf{b} = b_y \mathbf{e}_y$$

$$\mathbf{a}' = a_x \mathbf{e}_x = \mathbf{a}, \quad \mathbf{b}' = -b_y \mathbf{e}_y = -\mathbf{b}$$



(2) $a_y = 0$ and $b_x = \frac{1}{2}a_x$ (centered rectangular lattice)

Suppose that

$$\mathbf{a} = a_x \mathbf{e}_x, \quad \mathbf{b} = b_x \mathbf{e}_x + b_y \mathbf{e}_y$$

leading

to

$$\mathbf{a}' = a_x \mathbf{e}_x \quad \mathbf{b}' = b_x \mathbf{e}_x - b_y \mathbf{e}_y$$

We note that \mathbf{b}' must be a translation vector. Thus we set

$$\begin{aligned} \mathbf{b}' &= n_1 \mathbf{a} + n_2 \mathbf{b} \\ &= n_1 a_x \mathbf{e}_x + n_2 (b_x \mathbf{e}_x + b_y \mathbf{e}_y) \\ &= (n_1 a_x + n_2 b_x) \mathbf{e}_x + n_2 b_y \mathbf{e}_y \\ &= b_x \mathbf{e}_x - b_y \mathbf{e}_y \end{aligned}$$

or

$$n_1 a_x + n_2 b_x = b_x \quad \text{and} \quad n_2 = -1$$

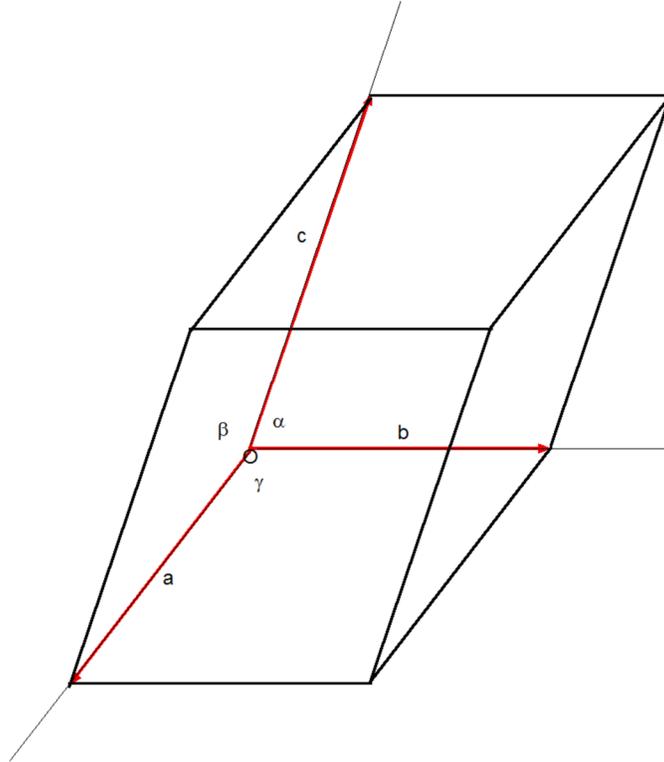
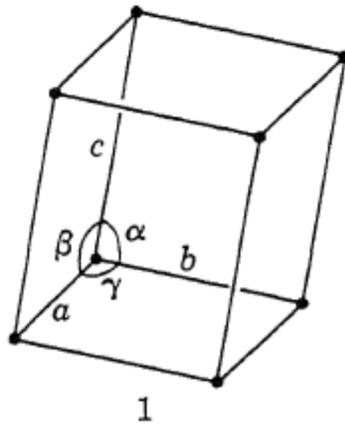


Fig. Definition of sides a (a_1), b (a_2), c (a_3), and angles α , β , and γ .

Triclinic

$$a_1 \neq a_2 \neq a_3$$

$$\alpha \neq \beta \neq \gamma$$

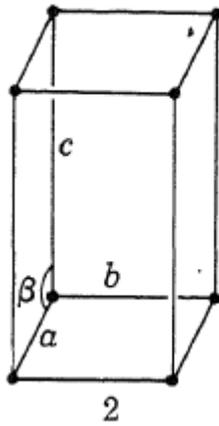


1. Triclinic, simple

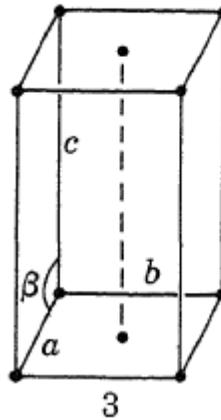
Monoclinic

$$a_1 \neq a_2 \neq a_3$$

$$\alpha = \gamma = 90^\circ \neq \beta$$



2. Monoclinic, simple

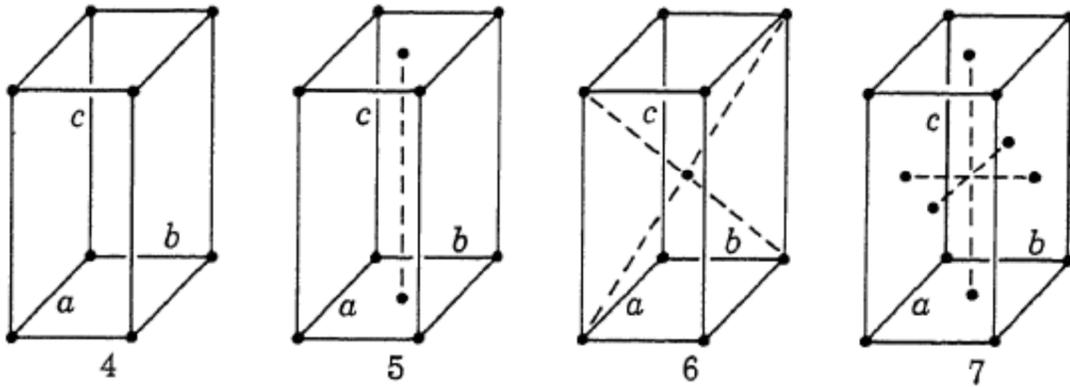


3. Monoclinic, base centered

Orthorhombic

$$a_1 \neq a_2 \neq a_3$$

$$\alpha = \beta = \gamma = 90^\circ.$$

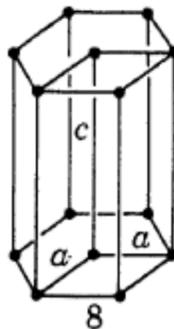


4. Orthorhombic, simple
5. Orthorhombic, base centered
6. Orthorhombic, body-centered (b.c.)
7. Orthorhombic, face-centered (f.c.)

Hexagonal

$$a_1 = a_2 \neq a_3$$

$$\alpha = \beta = 90^\circ, \gamma = 120^\circ.$$

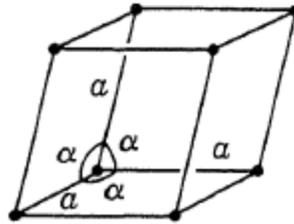


8. Hexagonal

Trigonal

$$a_1 = a_2 = a_3$$

$$\alpha = \beta = \gamma < 120^\circ, \neq 90^\circ.$$



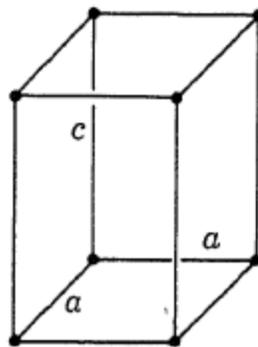
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9. Trigonal

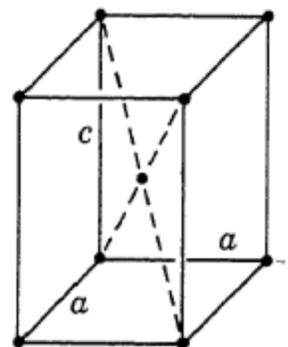
Tetragonal

$$a_1 = a_2 \neq a_3$$

$$\alpha = \beta = \gamma = 90^\circ.$$



10



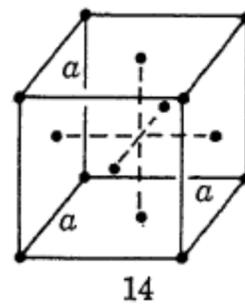
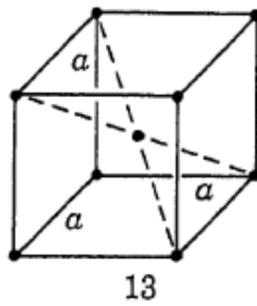
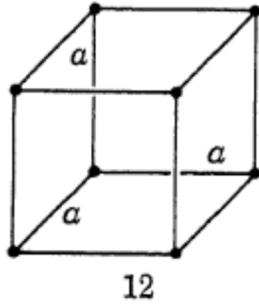
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10. Tetragonal , simple

11. Tetragonal, body-centered (b.c.)

Cubic

$$a_1 = a_2 = a_3$$
$$\alpha = \beta = \gamma = 90^\circ.$$



- 12. simple cubic (sc)
- 13. body-centered cubic (bcc)
- 14. face-centered cubic (fcc)

10. Simple cubic (sc)

The primitive cell is defined by the primitive translation vectors, \mathbf{a}_x , \mathbf{a}_y , and \mathbf{a}_z . There is only one lattice point.

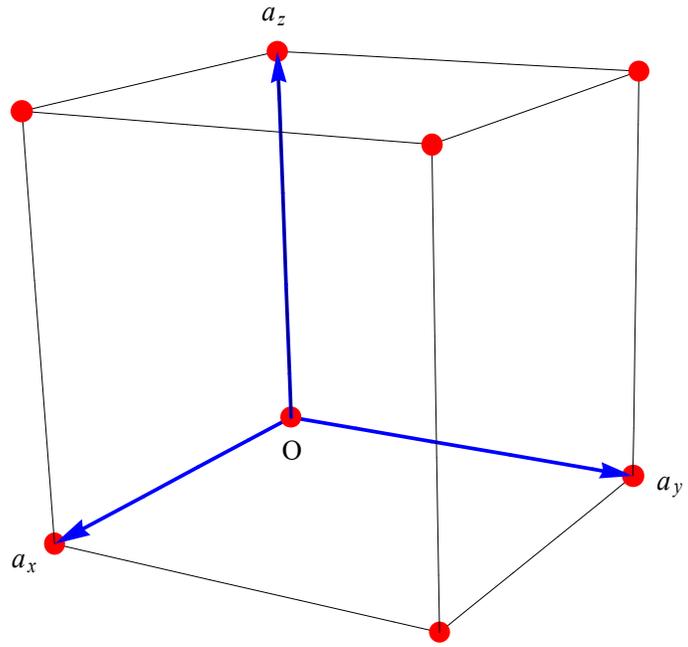


Fig. Structure of simple cubic (sc) lattice.

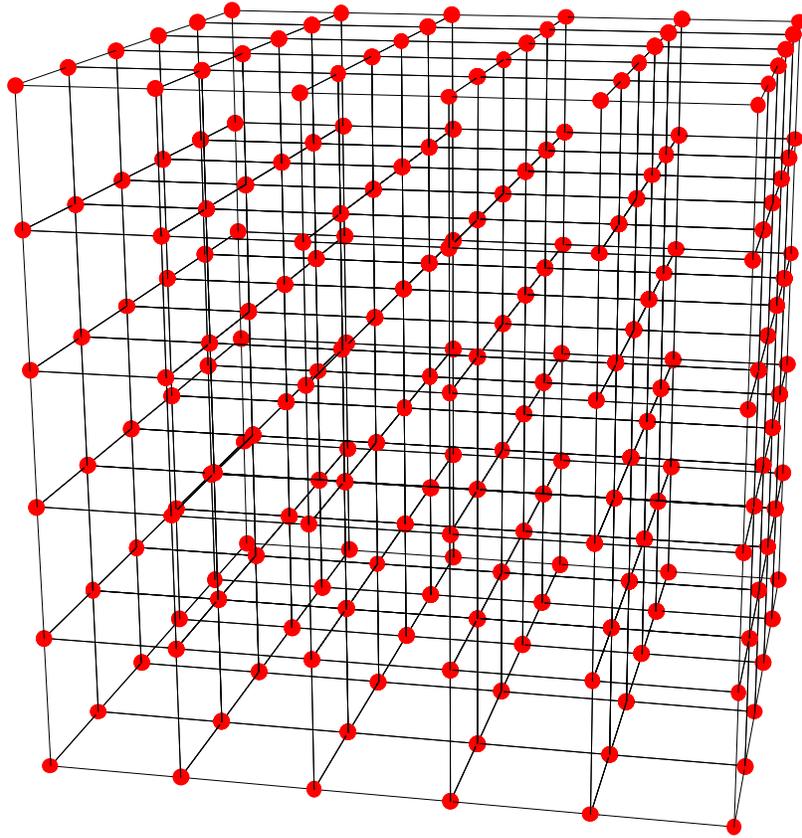


Fig. Building up of the 3D structure with sc lattice.

11. Face centered cubic (fcc) lattice

The crystal structure of the fcc is given below.

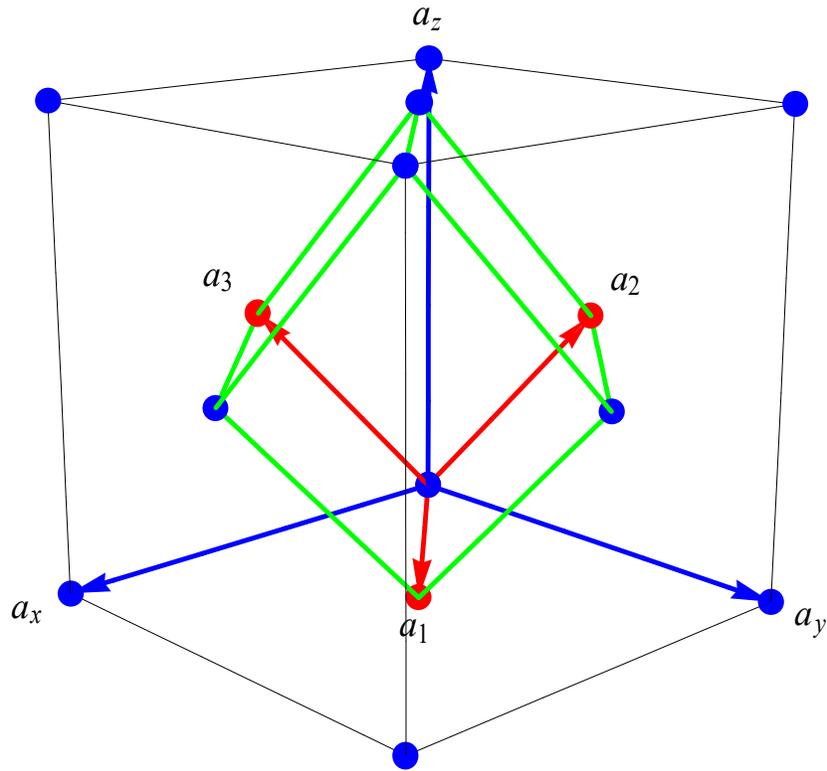


Fig. Primitive cell ($\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$) and conventional cell ($\mathbf{a}_x, \mathbf{a}_y, \mathbf{a}_z$) for the fcc lattice.

Conventional cell

There are four lattice points in this cell,

$$8 \times \frac{1}{8} + 6 \times \frac{1}{2} = 1 + 3 = 4.$$

$\mathbf{a}_x, \mathbf{a}_y,$ and \mathbf{a}_z are the translation vectors of this cell.

Primitive cell:

There is only one lattice point of this cell. $\mathbf{a}_1, \mathbf{a}_2,$ and \mathbf{a}_3 are the primitive translation vectors.

$$\mathbf{a}_1 = \frac{a}{2}(1,1,0), \quad \mathbf{a}_2 = \frac{a}{2}(0,1,1), \quad \mathbf{a}_3 = \frac{a}{2}(1,0,1)$$

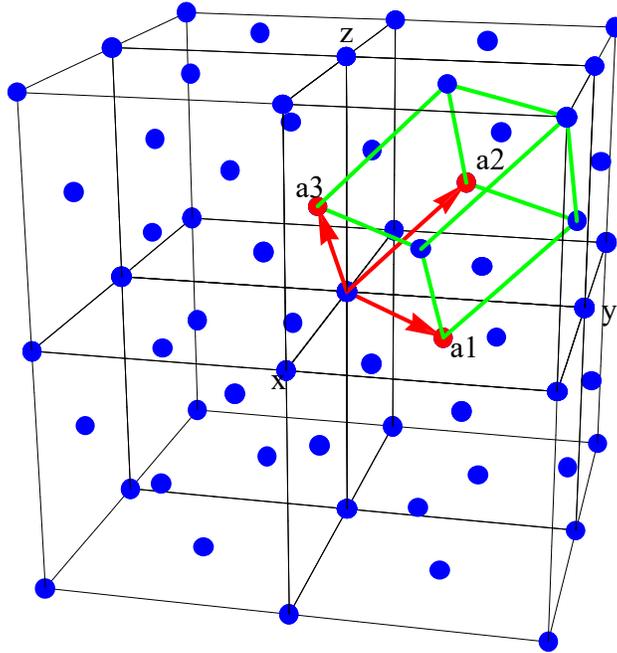


Fig. Building up of 3D structure with the bcc lattice.

$$\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3) = \frac{a^3}{8} \begin{vmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{vmatrix} = \frac{a^3}{8} \times 2 = \frac{a^3}{4}$$

$$\mathbf{a}_x \cdot (\mathbf{a}_y \times \mathbf{a}_z) = a^3 \begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix} = a^3 \times 1 = a^3$$

12. Body-centered cubic (bcc) lattice

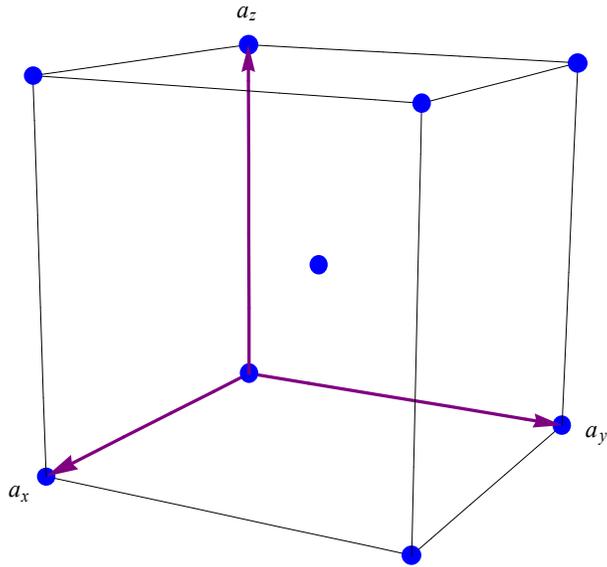


Fig. bcc lattice. Conventional cell. There are two lattice points. \mathbf{a}_x , \mathbf{a}_y and \mathbf{a}_z are the translation vectors.

This is a conventional cell since there are two lattice points in the cell,

$$8 \times \frac{1}{8} + 1 = 2.$$

The conventional cell consists of a lattice point plus a basis. The vector \mathbf{a}_x , \mathbf{a}_y and \mathbf{a}_z are the translation vectors of the conventional cell.

The primitive cell consists of the primitive translation vectors \mathbf{a}_1 , \mathbf{a}_2 , and \mathbf{a}_3 . There is only one lattice point in this cell.

$$\mathbf{a}_1 = \frac{a}{2}(1, 1, -1), \quad \mathbf{a}_2 = \frac{a}{2}(-1, 1, 1), \quad \mathbf{a}_3 = \frac{a}{2}(1, -1, 1).$$

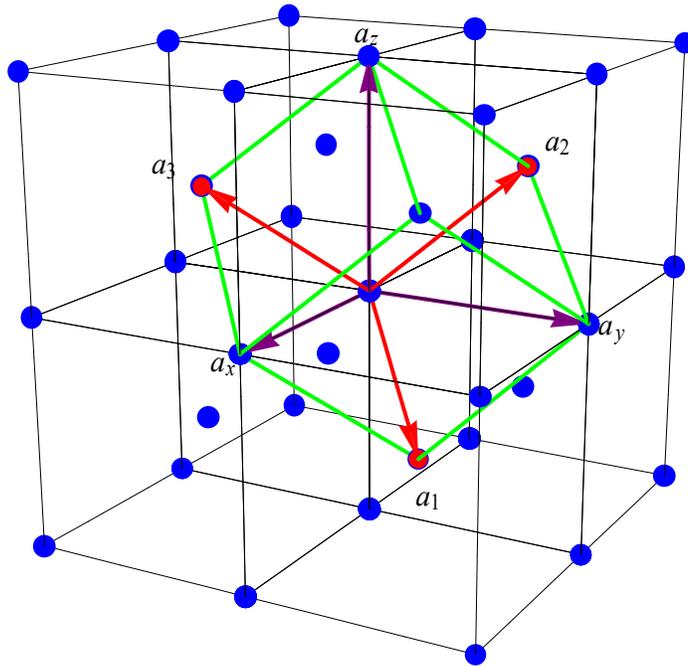


Fig. Primitive cell. There is only one lattice point at the body center. \mathbf{a}_1 , \mathbf{a}_2 , and \mathbf{a}_3 are the primitive translation vectors.

$$\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3) = \frac{a^3}{8} \begin{vmatrix} 1 & 1 & -1 \\ -1 & 1 & 1 \\ 1 & -1 & 1 \end{vmatrix} = \frac{a^3}{8} \times 4 = \frac{a^3}{2}$$

$$\mathbf{a}_x \cdot (\mathbf{a}_y \times \mathbf{a}_z) = a^3 \begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix} = a^3 \times 1 = a^3$$

13. Hexagonal lattice

A hexagonal lattice is shown below. This structure does not occur among the elements, except as the starting point of the hexagonal close-packed structure. Its primitive vectors are \mathbf{a}_1 , \mathbf{a}_2 , and \mathbf{a}_3 .

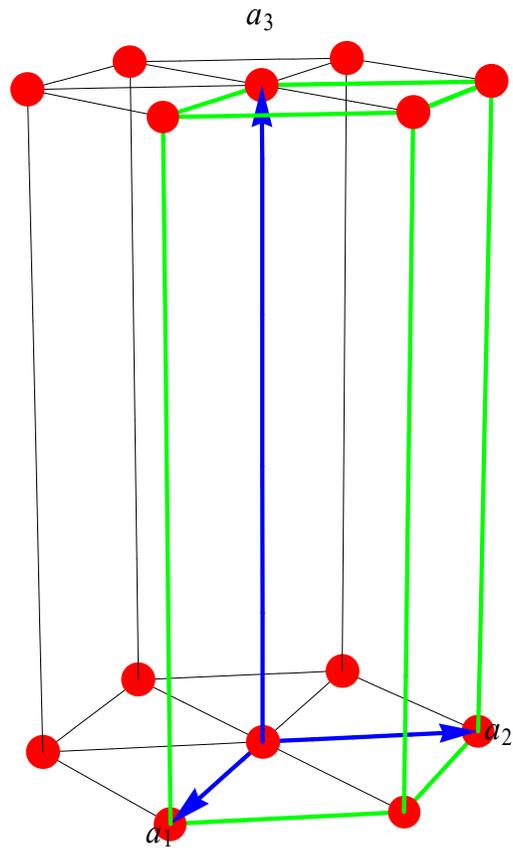


Fig. Hexagonal lattice. $a_1 = a_2 = a$. $\angle a_1, a_2 = 120^\circ$. $a_3 = c$.

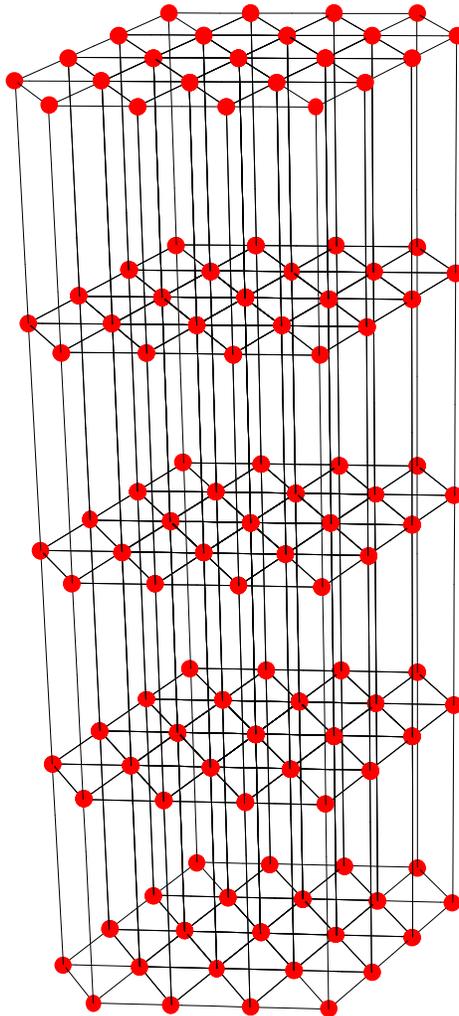


Fig. Building up of the 3D structure with the hexagonal lattice.

14. Fundamental types of lattices

The symmetry operations of a crystal carry the crystal structure into itself.

Lattice translation operator

Rotation reflection = point operation

((Rotation))

A typical symmetry rotation is that of rotation about an axis that passes through a lattice point.

1

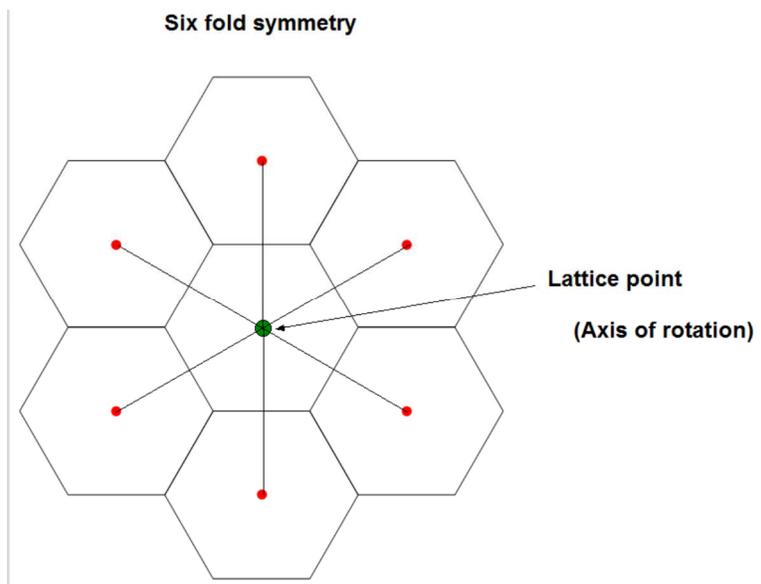
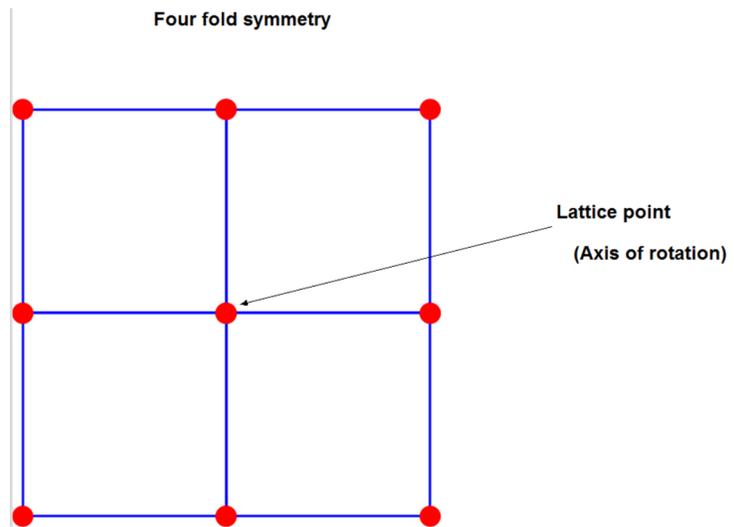
one

$\theta = 2\pi$

2	(diad axis)	two fold rotation	$\theta = 2\pi / 2 = \pi$
3	(triad axis)	three fold rotation	$\theta = 2\pi / 3$
4	(tetrad axis)	four fold rotation	$\theta = 2\pi / 4 = \pi / 2$
6	(hexad axis)	six fold rotation	$\theta = 2\pi / 6$

We can not find a lattice that goes into itself under other rotation such as by $\theta = 2\pi / 7$ or $\theta = 2\pi / 5$.

((Example))



((Quasi crystal)) **Five-fold symmetry ?**

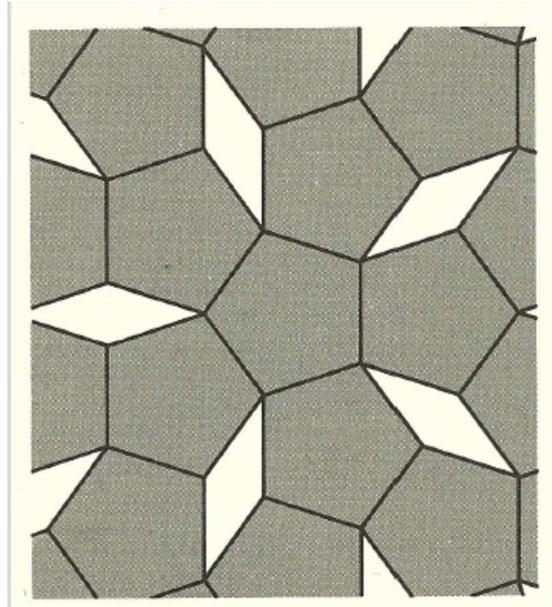
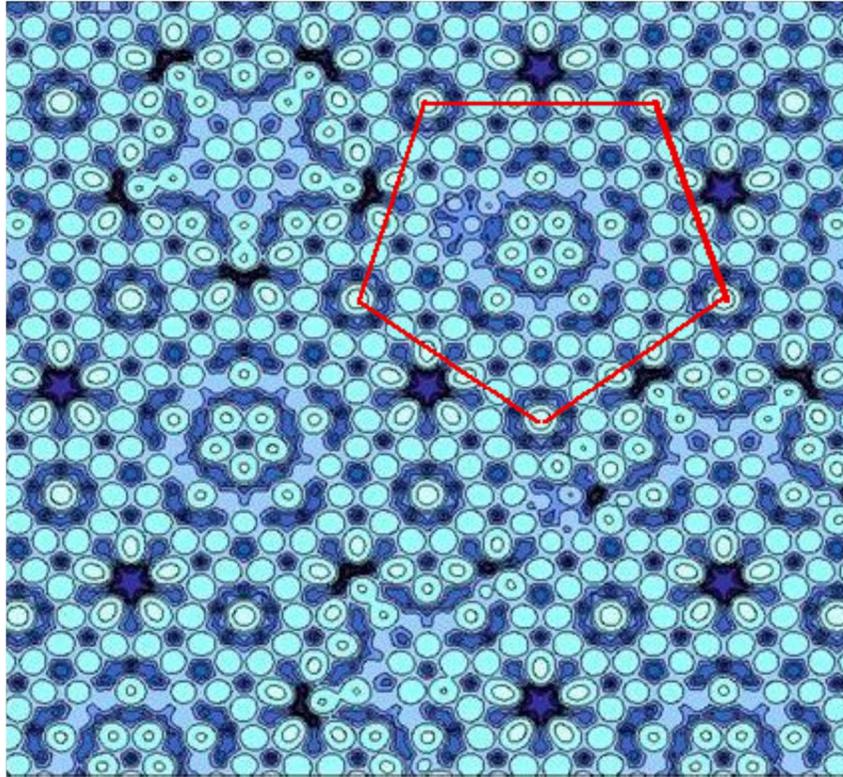


Fig. A five-fold axis of symmetry cannot exist in a lattice because it is not impossible to fill all space with a connected array of pentagons. As shown in this figure we give an example of regular pentagonal packing which does not have the translational invariance of a lattice. (C. Kittel, ISSP 4th edition, Chapter 1, p.13, Fig.9a)



The pentagons do not fit together to fill all space, showing that we cannot combine fivefold point symmetry with the required translational periodicity

((Note))

On April 8, 1982, while on sabbatical at the U.S. National Bureau of Standards in Washington, D.C., Shechtman discovered the icosahedral phase, which opened the new field of quasiperiodic crystals. He was awarded the 2011 Nobel Prize in Chemistry for "the discovery of quasicrystals"

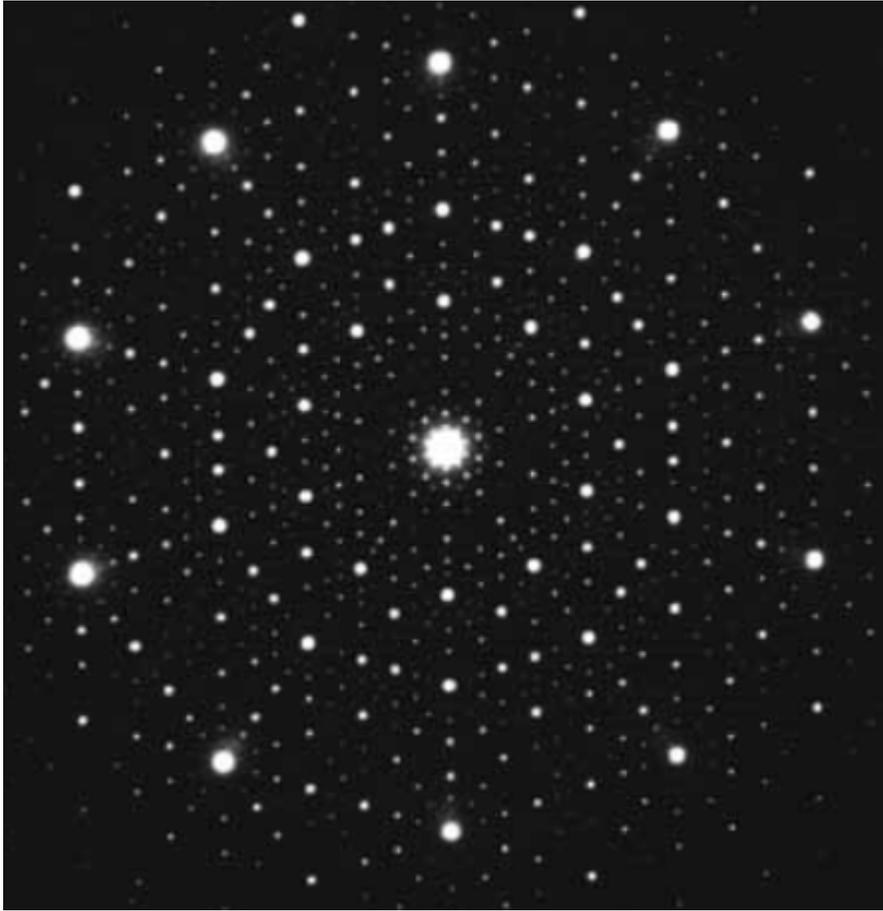
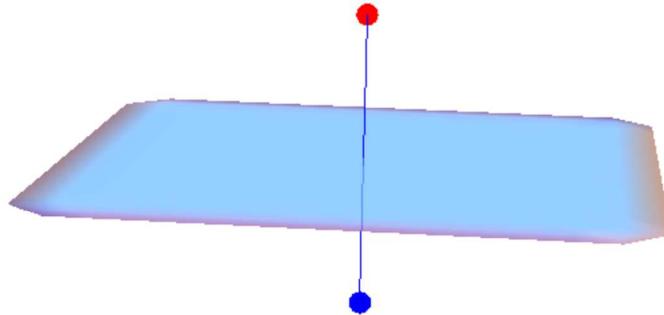


Fig. The electron diffraction pattern from an icosahedral quasi crystal contains perfect pentagons. (from Nobel lecture by Prof. D. Shechtman).

http://www.rsc.org/images/Nobel%20Prize%20-%20Quasicrystals%20Scoop%20Prize_tcm18-209332.pdf

(i) Mirror symmetry

We can have mirror reflection (m) about a plane through a lattice point (reflection plane).



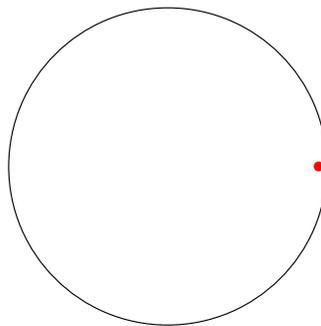
(ii) Inversion

The Inversion operation is composed of a rotation of π followed by reflection in a plane normal to the rotation axis. The total effect is to replace

$$r \rightarrow -r.$$

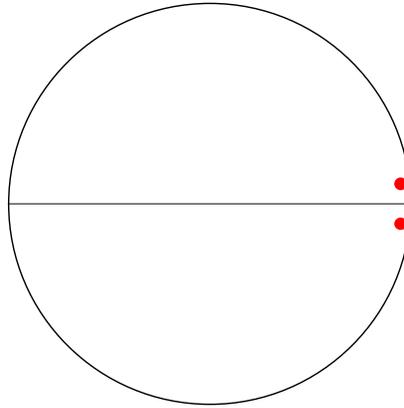
(iii) Point group

(a) 1-fold axis: rotation of 2π 1



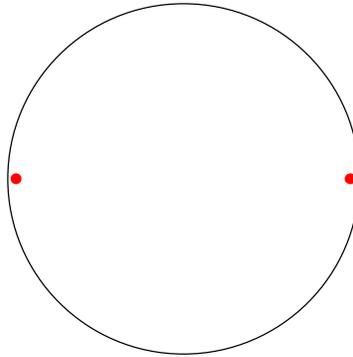
(b) Mirror plane

"1*m*"



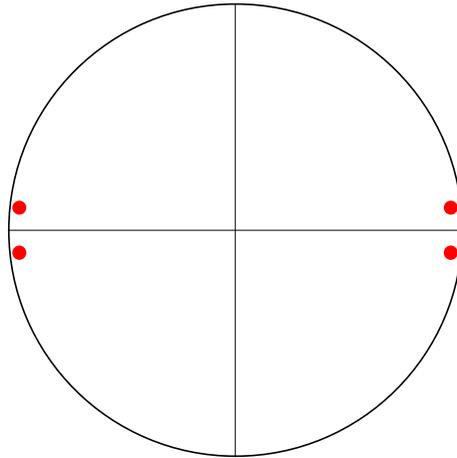
(c) Two fold axis; rotation of π

"2"



(d) A two-fold axis. One mirror plane

"2*mm*"



There is automatically a second mirror plane normal to the first mirror plane.

15. Fundamental types of lattices

((Mathematical interest))

We can find a lattice that goes into itself under the rotation of $2\pi/n$ with only $n = 1, 2, 3, 4,$ and 6 .

((Proof))

Suppose that the axis of rotation is perpendicular to the primitive translation vector \mathbf{T} . We will prove later that the axis of the rotation should be the primitive translation vector.

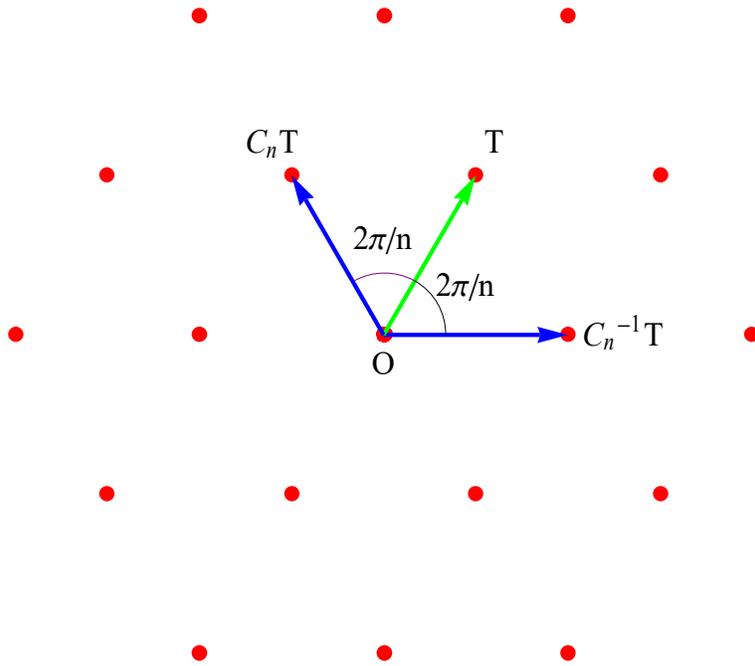


Fig. \mathbf{T} : primitive translation vector. O is the axis of rotation. The axis of rotation is also assumed to be one of the primitive translation vector (this will be proved later). The direction of the axis of rotation is out of the page.

C_n is the rotation of $2\pi/n$ around the axis and C_n^{-1} is the rotation of $-2\pi/n$ around the axis, respectively. A lattice goes into itself under the rotation of $2\pi/n$ with only n . This means that $C_n\mathbf{T}$ and $C_n^{-1}\mathbf{T}$ are also primitive translation vectors. Then the vector sum given by

$$C_n\mathbf{T} + C_n^{-1}\mathbf{T} = 2T \cos\left(\frac{2\pi}{n}\right)\mathbf{n} = 2T \cos\left(\frac{2\pi}{n}\right),$$

must be a translation vector and be integer times \mathbf{T} . So the value of n can be obtained as

$$n = 1, 2, 3, 4, \text{ and } 6.$$

since $2 \cos\left(\frac{2\pi}{n}\right) = 2$ for $n = 1$, $2 \cos\left(\frac{2\pi}{n}\right) = 0$ for $n = 2$, $2 \cos\left(\frac{2\pi}{n}\right) = 1$ for $n = 3$, $2 \cos\left(\frac{2\pi}{n}\right) = 0$ for $n = 4$, and $2 \cos\left(\frac{2\pi}{n}\right) = -2$.

We now assume that the primitive translation vector \mathbf{T}_1 is not perpendicular to the axis of rotation. Suppose that this vector \mathbf{T}_1 is rotated around the axis of rotation by the angle $2\pi/n$ (C_n is the rotation of $2\pi/n$ around the axis). After the repetition of this process by n times, we get new primitive translation vectors, $\mathbf{T}_2, \mathbf{T}_3, \dots, \mathbf{T}_n = \mathbf{T}_1$, in order, where n is an integer. The figure shows the case for $n = 6$.

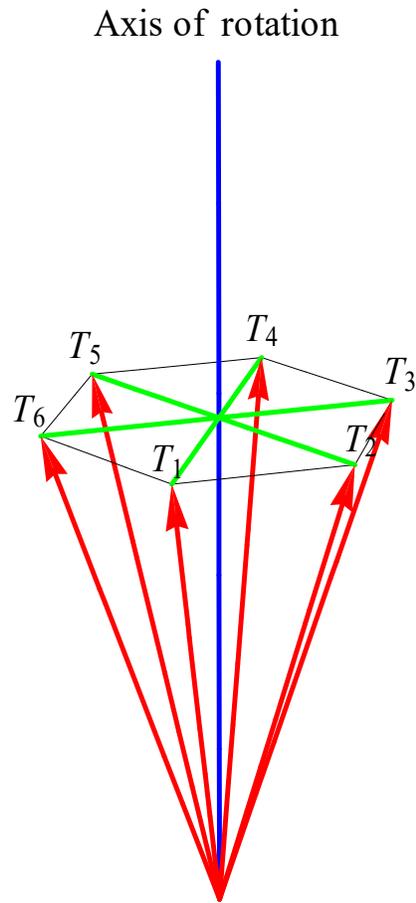


Fig. Rotation of the primitive translation vector around the axis of rotation ($C_{n=6}$). $\mathbf{T}_1, \mathbf{T}_2, \dots,$ and \mathbf{T}_6 are the primitive translation vectors. The vector $(\mathbf{T}_n - \mathbf{T}_{n+1})$ ($n = 1, 2, \dots, 6$) are also the primitive translation vector.

$$|\mathbf{T}_1| = |\mathbf{T}_2| = |\mathbf{T}_3| = \dots = |\mathbf{T}_n|.$$

Note that $T_1 + T_2 + T_3 + \dots + T_n$ is also translation vectors and is parallel to the axis of rotation. $T_{12} = T_1 - T_2$, $T_{23} = T_2 - T_3$, $T_{34} = T_3 - T_4$, ..., are the primitive translation vectors and are perpendicular to the axis of rotation. Then the axis of the rotation is the primitive translation vector. There always exists the primitive translation vectors which is perpendicular to the axis of rotation (which is also the primitive translation vector).

In conclusion, the rotation of $2\pi/n$ with only $n = 5$ does not exist in the crystals.

((Note)) In spite of the above theorem, a quasi-crystal shows the $n = 5$ symmetry.

16. NaCl structure

The space lattice is fcc. Na^+ and Cl^- ions are alternately arranged at the lattice points of a sc lattice. Each ion is surrounded by 6 nearest neighbors of the opposite charge.

Conventional cell:

$$\text{Cl}^-: \quad 1 + 6 \times \frac{1}{2} = 4$$

$$\text{Na}^+: \quad 12 \times \frac{1}{4} + 1 = 4$$

There are four units of NaCl in each unit cube, with atoms in the positions,

Cl^- :

$$(0,0,0), \quad (1/2,1/2,0), \quad (1/2,0, 1/2), \quad (0, 1/2, 1/2)$$

Na^+ :

$$(1/2,1/2,1/2), \quad (0,0,1/2) \quad (0,1/2,0), \quad (1/2,0,0)$$

The basis has one Cl^- ion at $(0,0,0)$ and one Na^+ ion at $(1/2, 1/2, 1/2)$.

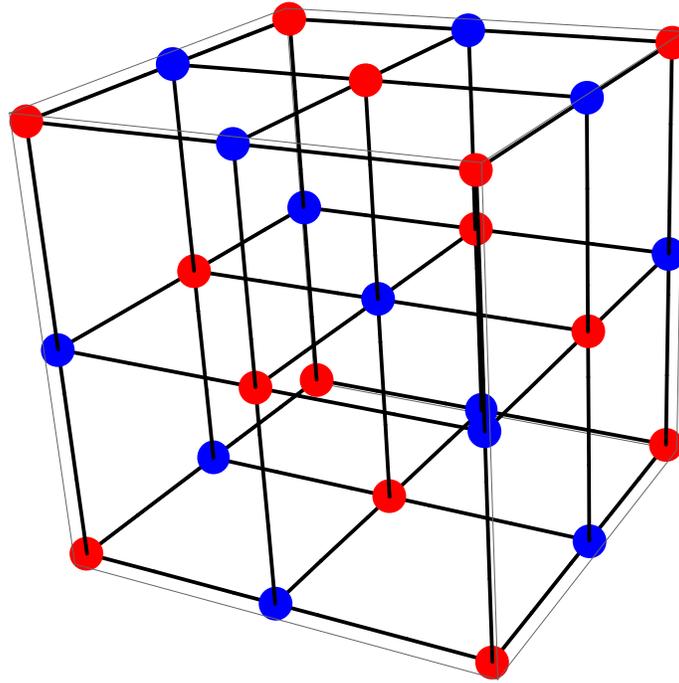


Fig. NaCl structure. Cl^- (red circles) and Na^+ (blue circles). $a = 5.63 \text{ \AA}$.

17. CsCl structure

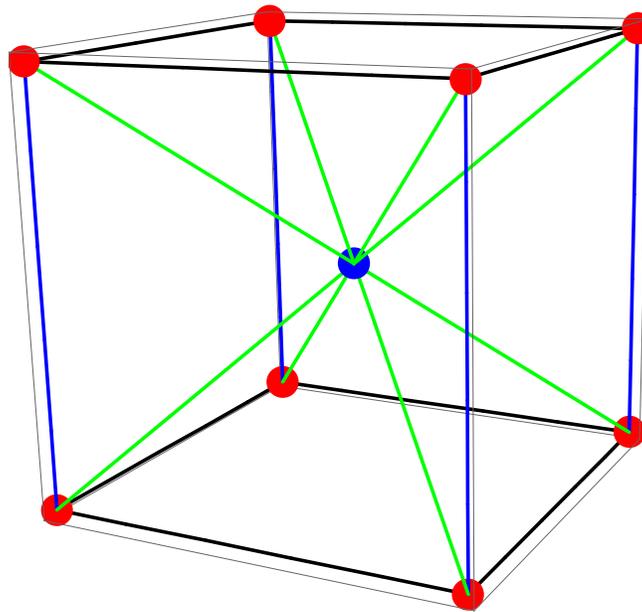
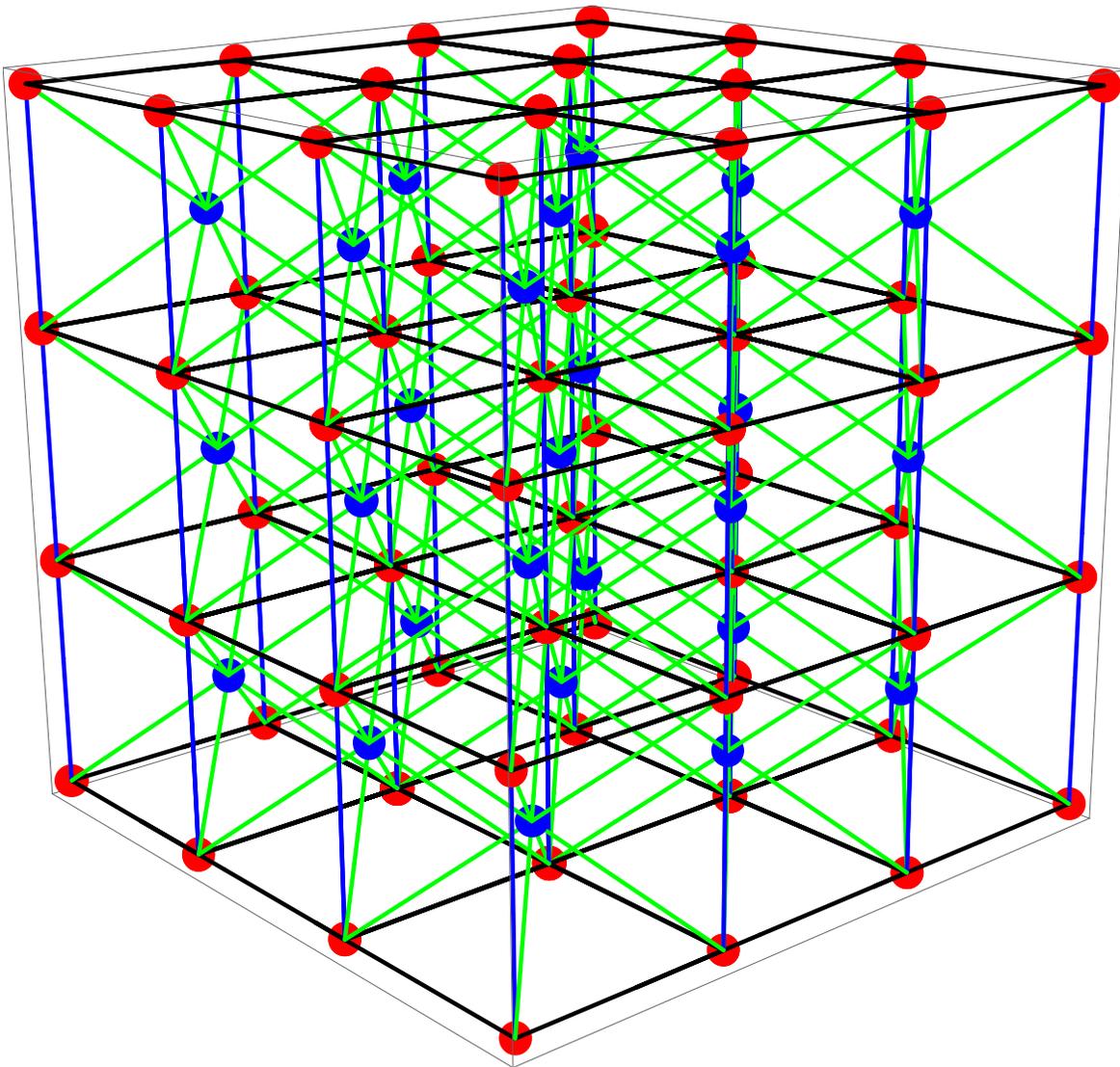


Fig. CsCl structure. simple cubic (primitive cell). $a = 4.11 \text{ \AA}$. Cs^+ ion (red). Cl^- ion (blue).

Each atom may be viewed as at the center of a cube of atoms of the opposite kind. The number of the nearest neighbor (n. n.) or co-ordination number is $z = 8$. The space lattice is **simple cubic (primitive cell)**. The basis has one Cs^+ ion at $(0,0,0)$ and one Cl^- ion at $(1/2, 1/2, 1/2)$.



18. Hexagonal close-packed (hcp) structure

The in-plane structure is hexagonal symmetry. There are several types of stacking sequences along the plane.

- (1) AAAAA... stacking
- (2) ABABAB... stacking
- (3) ABCABC stacking fcc (111) plane.

The hcp structure has the primitive cell of the hexagonal lattice, but with a basis of two atoms.

$$a_1 = a_2 = a, \quad \angle a_1, a_2 = 120^\circ$$

A basis of two atoms at

$$\mathbf{r} = 0, \quad \mathbf{r} = \frac{2\mathbf{a}_1 + \mathbf{a}_2}{3} + \frac{\mathbf{a}_3}{2}$$

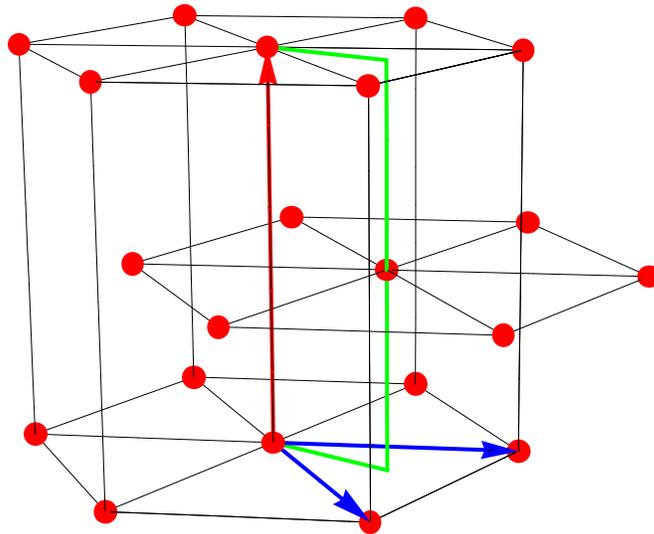


Fig. Hcp structure with $c/a = 1.633$.

The ratio c/a for the hcp of spheres has the value

$$\frac{c}{a} = \sqrt{\frac{8}{3}} = 1.633.$$

It is usual to refer to crystals as hcp even if the actual c/a ratio departs somewhat from this theoretical value. The number of the nearest-neighbor atoms is 12 for both hcp and fcc.

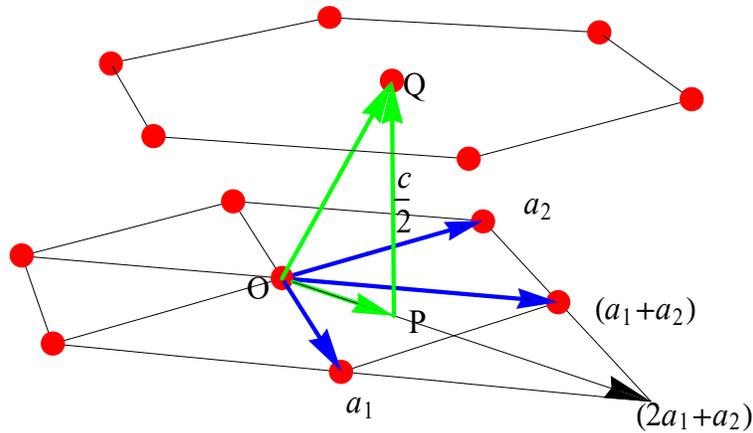


Fig. Hexagonal close-packed lattice. Primitive cell has $a_1 = a_2 = a$, with an included angle 120° . The c -axis (a_3) is normal to a_1 and a_2 . The ideal hcp structure has $c = 1.633 a$. $\vec{OP} = \frac{2\mathbf{a}_1 + \mathbf{a}_2}{3}$. $\vec{OQ} = \frac{2\mathbf{a}_1 + \mathbf{a}_2}{3} + \frac{\mathbf{a}_3}{2}$

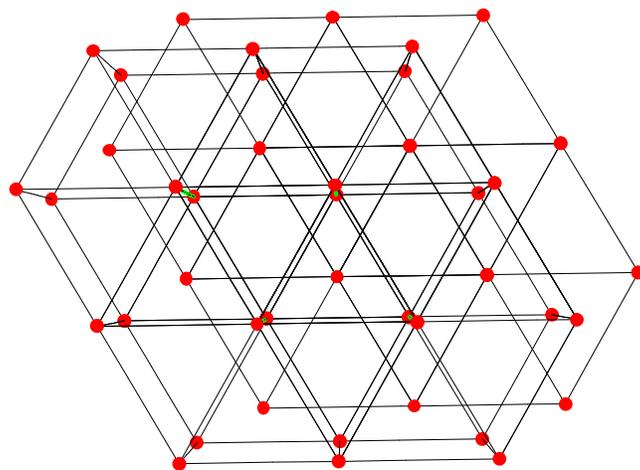


Fig. Top view of an hcp lattice. The ABAB.... stacking. This figure made from the Graphics3D of the Mathematica, leading to incomplete superposition of points.

((Structure of graphite))

The graphite has a AB stacking sequence along the c axis. The lattice constants of graphite are given by $a_1 = a_2 = a = 2.46 \text{ \AA}$, $c = 6.70 \text{ \AA}$.

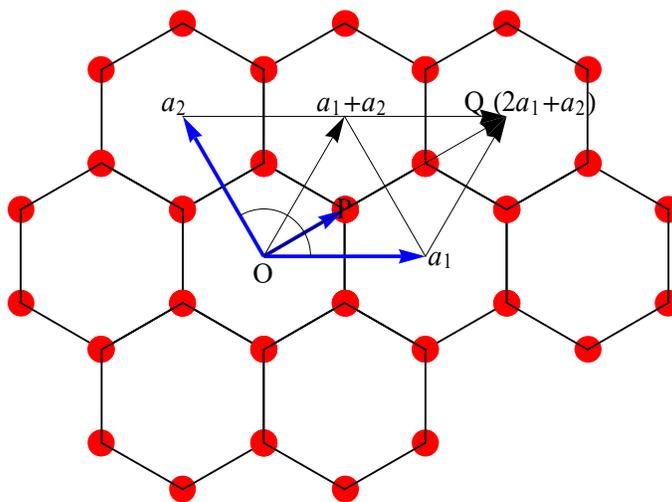


Fig. The in-plane structure of the A and B layers in the AB stacking sequence for the graphite. The lattice point of the B layer is at the point P, while the lattice point of the A layer is at the point O. $\overline{OP} = \frac{2\mathbf{a}_1 + \mathbf{a}_2}{3}$

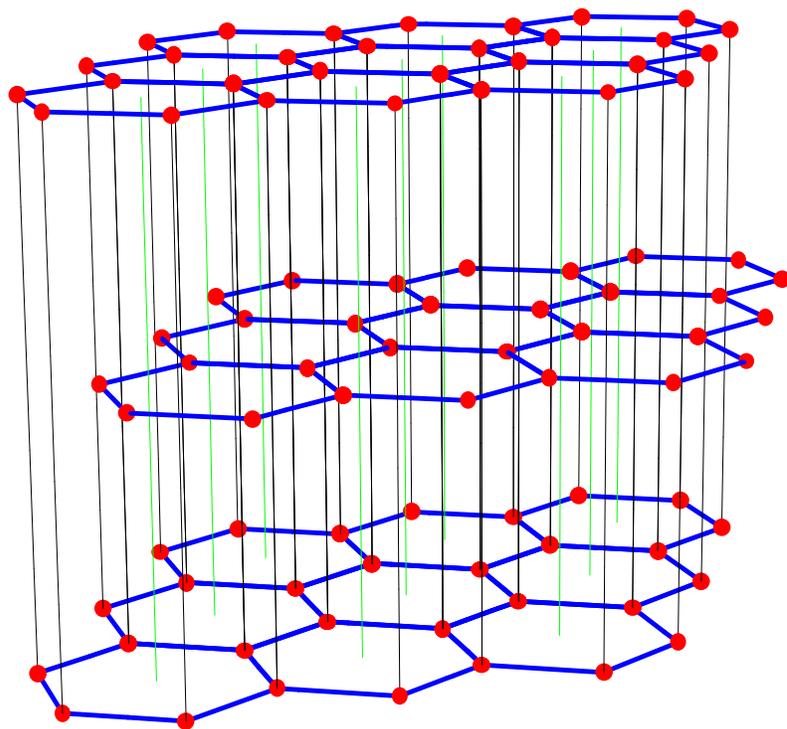
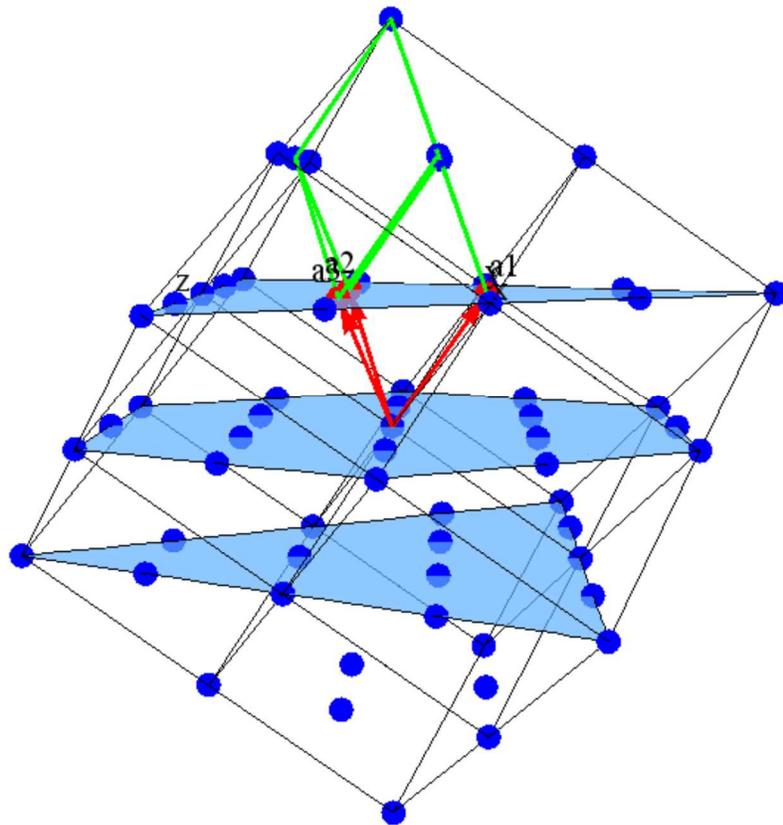


Fig. Graphite lattice, which has ABAB stacking sequence along the c axis.



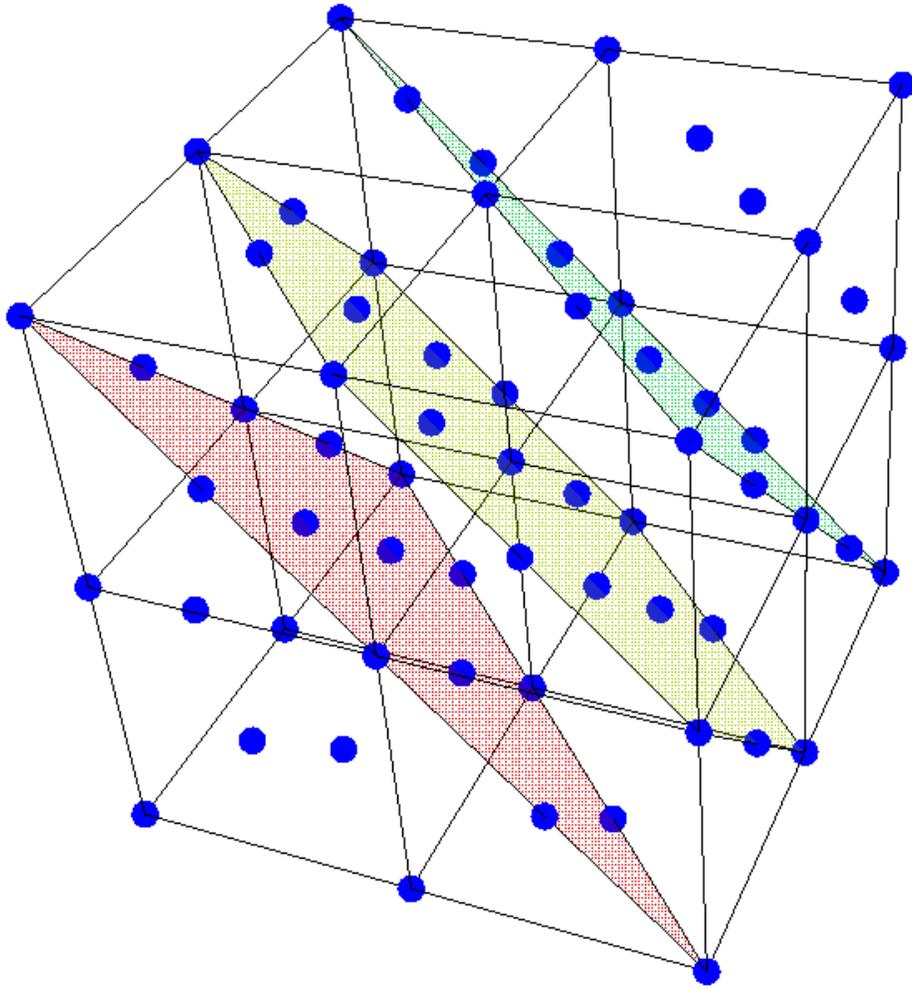


Fig. (111) plane of the fcc structure. The close-packed layers of the fcc structure has the stacking sequence ABCABC.....

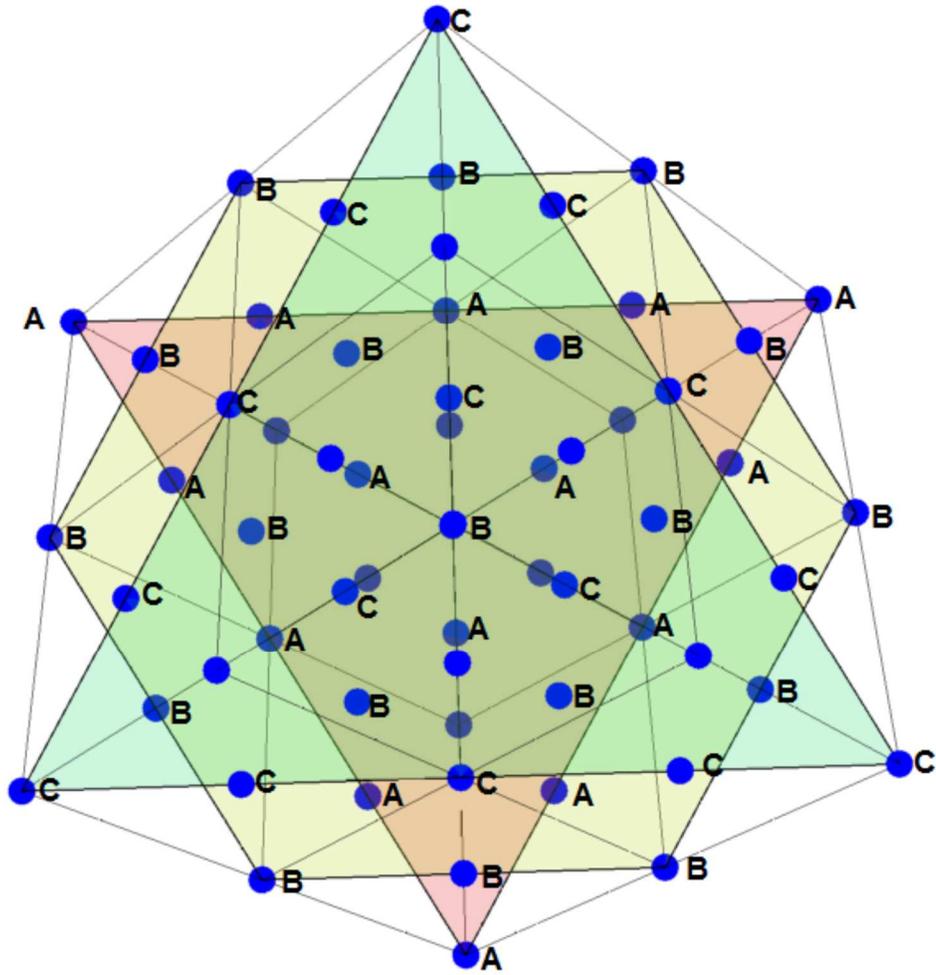


Fig. Top view of the fcc lattice viewed from (111) direction. This figure made from the Graphics3D of the Mathematica, leading to incomplete superposition of points.

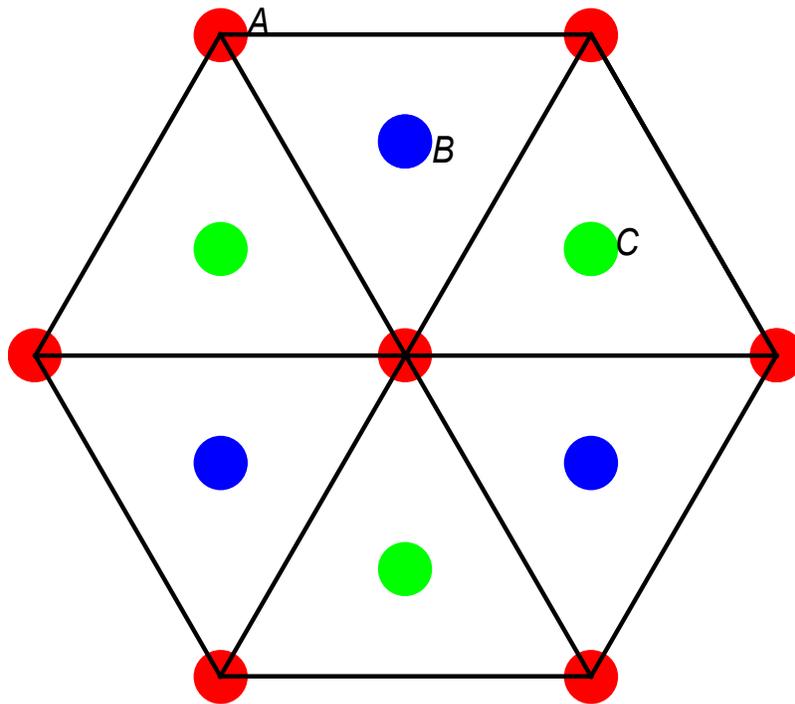


Fig. Ideal case. Top view of the fcc lattice viewed from (111) direction.

19. Diamond structure

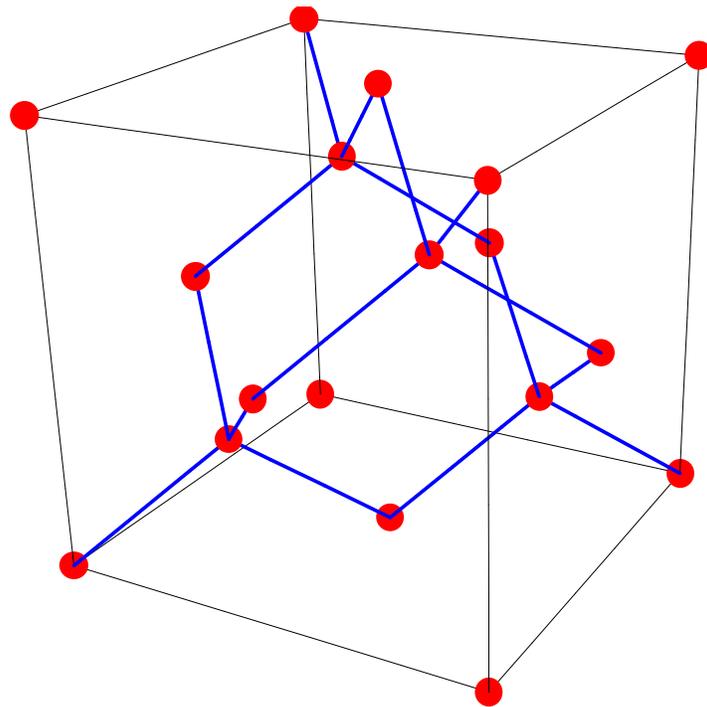


Fig. Crystal structure of diamond showing the tetrahedral bond arrangement.

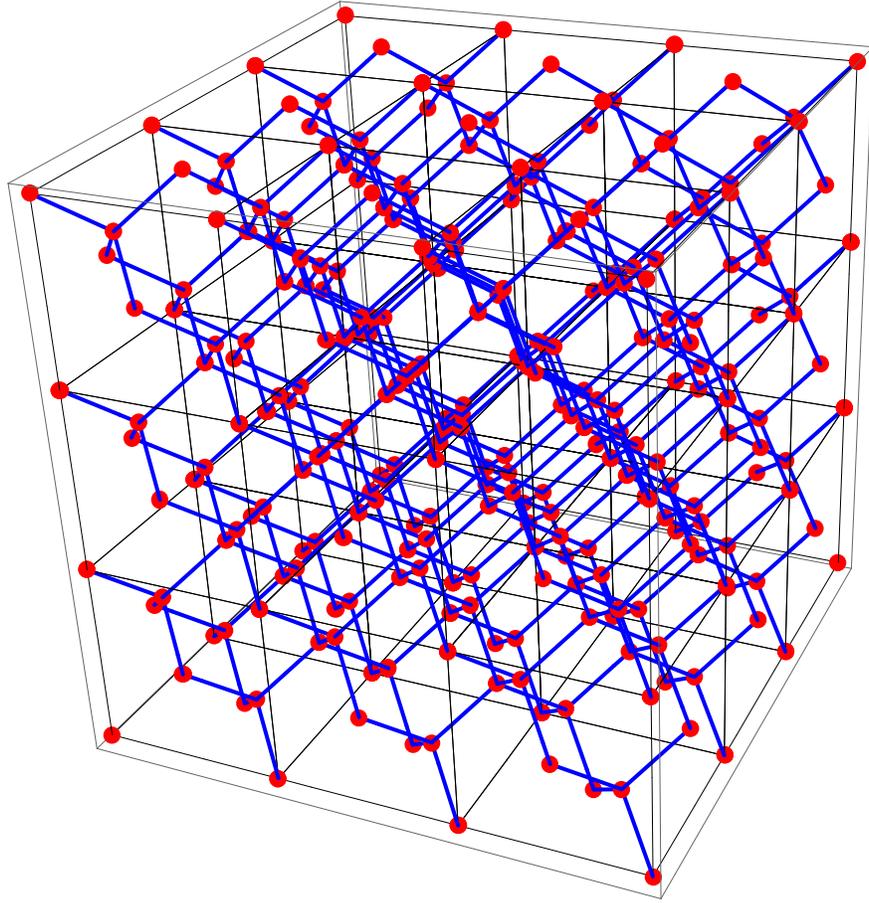
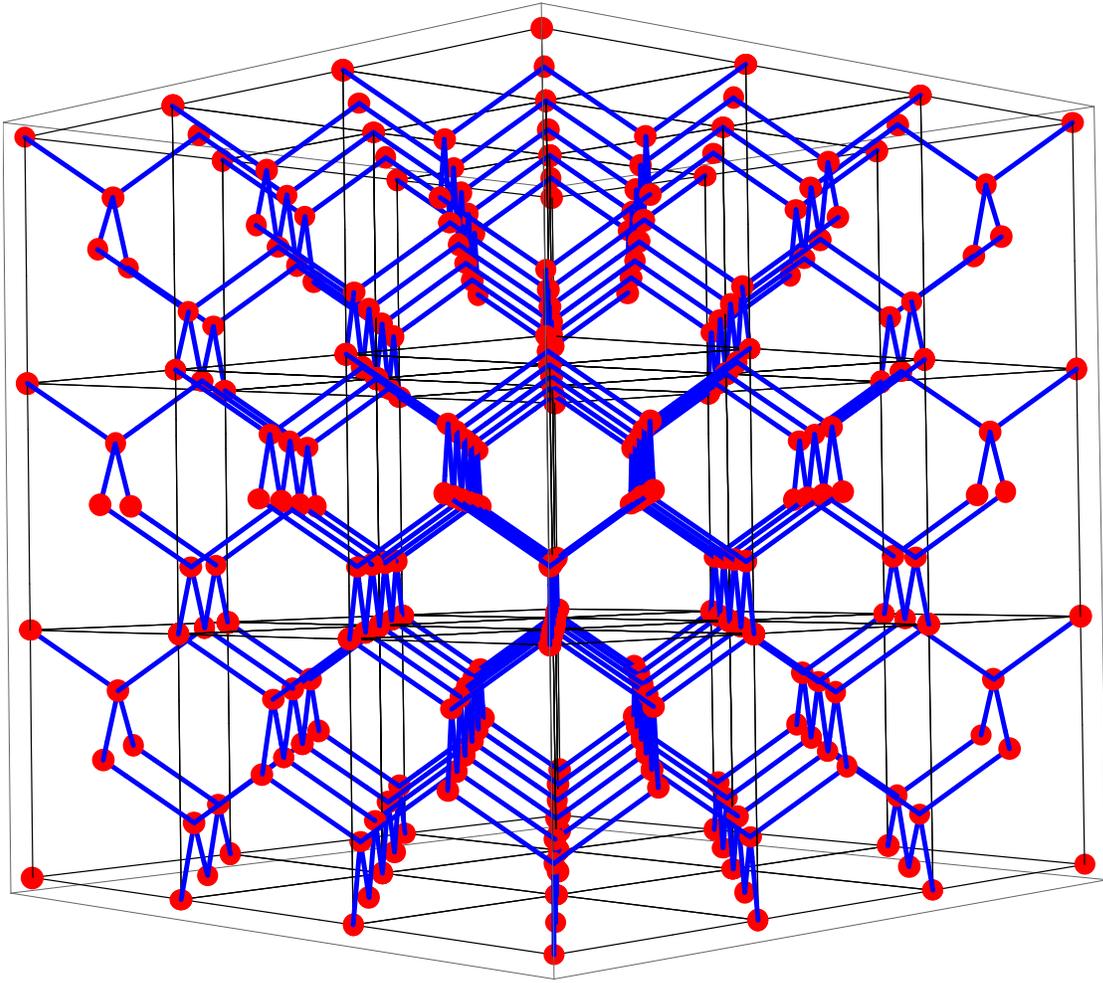


Fig. Diamond structure



20. ZnS structure

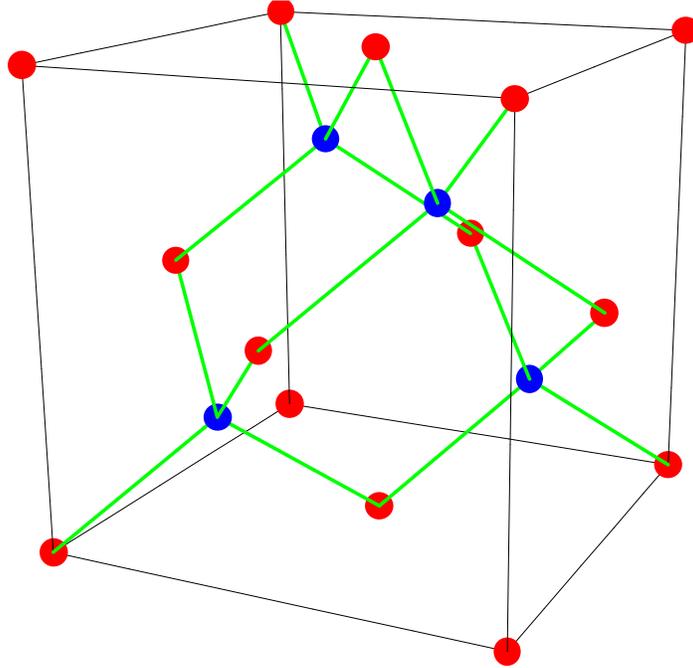


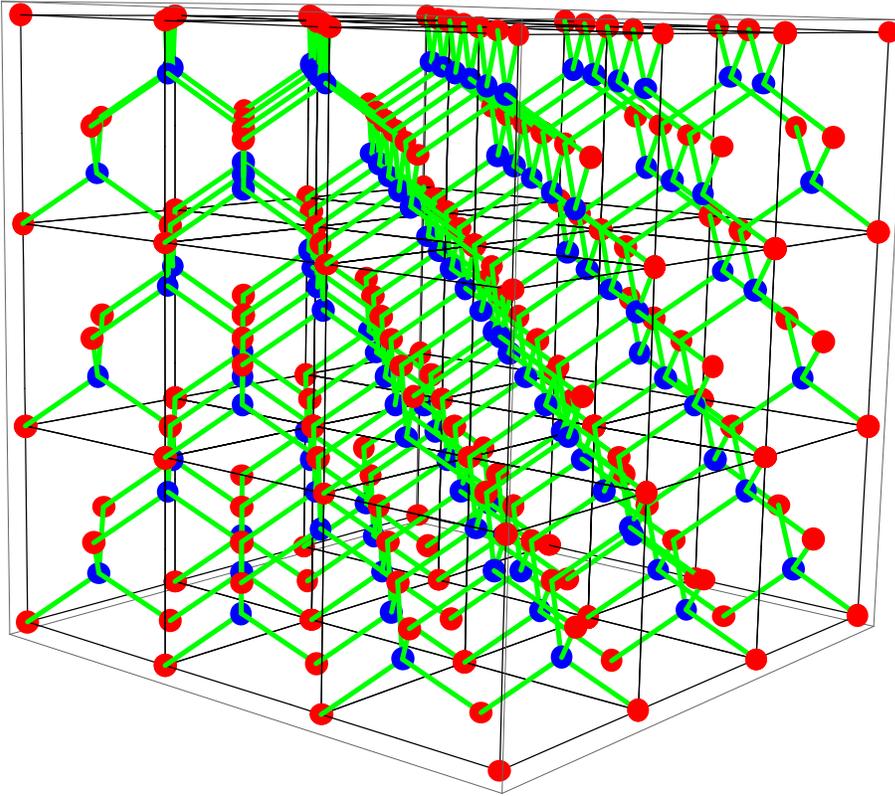
Fig. Crystal structure of ZnS. Zn (red circles). S (blue circles).

The conventional cell is cubic.

Zn: $(0, 0, 0), (0, 1/2, 1/2), (1/2, 0, 1/2), (1/2, 1/2, 0)$: red circles.

S: $(1/4, 1/4, 1/4), (1/4, 3/4, 3/4); (3/4, 1/4, 3/4), (3/4, 3/4, 1/4)$ black circles

The lattice is fcc. There are four molecules of ZnS per conventional cell.



21. Definition of Miller indices

We often find it necessary to describe a particular crystallographic plane or, a particular direction within a real 3D crystal. Crystal planes are usually described by their Miller indices. Suppose that a plane intercepts at

$$p_1 \mathbf{a}_1 = \frac{n}{h} \mathbf{a}_1, \quad p_2 \mathbf{a}_2 = \frac{n}{k} \mathbf{a}_2, \quad p_3 \mathbf{a}_3 = \frac{n}{l} \mathbf{a}_3,$$

on the axes of \mathbf{a}_1 , \mathbf{a}_2 , \mathbf{a}_3 . The plane form by these three vectors is called a (hkl) plane, when

$$h = \frac{n}{p_1}, \quad k = \frac{n}{p_2}, \quad l = \frac{n}{p_3},$$

where h , k , and l are integers, and n is integer chosen to get the smallest three integers: (hkl) . These indices (hkl) may denote a single phase or a set of parallel planes with the index n . If a plane cuts an axis on the negative side of the origin, the corresponding index is negative, indicated by placing a minus sign above the index $(h\bar{k}l)$.

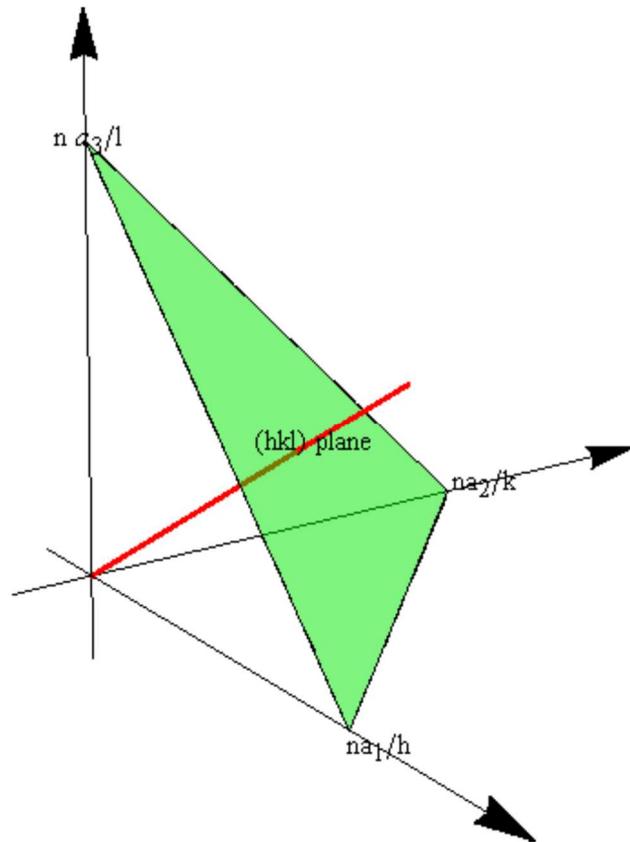


Fig. Definition of (hkl) plane where h , k , and l are the smallest three integers. n is integer and denotes the family of the (hkl) planes.

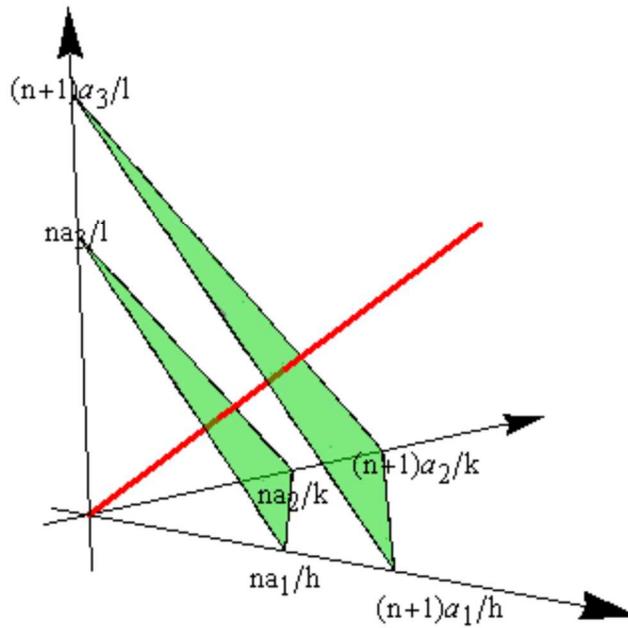


Fig. The family of (hkl) planes with index n , where n is an integer. The (hkl) plane with the index n intercepts at $na_1/h, na_2/k, na_3/l$. As will be described in the next chapter, $\mathbf{G}(h, k, l)$ (denoted by red line) is the reciprocal lattice vector. This vector \mathbf{G} is normal to the (hkl) plane.

22. Example-1

We consider the plane intercepts the a_1, a_2, a_3 axes at $3a_1, 2a_2, 2a_3$.

$$\frac{n}{h} = 3, \quad \frac{n}{k} = 2, \quad \frac{n}{l} = 2$$

or

$$h = \frac{n}{3}, \quad k = \frac{n}{2}, \quad l = \frac{n}{2}$$

Note that h, k, l and n are integers. When $n = 6$, we have a set of integers (hkl) ,

$$h = 2, \quad k = 3, \quad l = 3.$$

Then we can conclude that the plane is described by a miller indices (233) with $n = 6$.

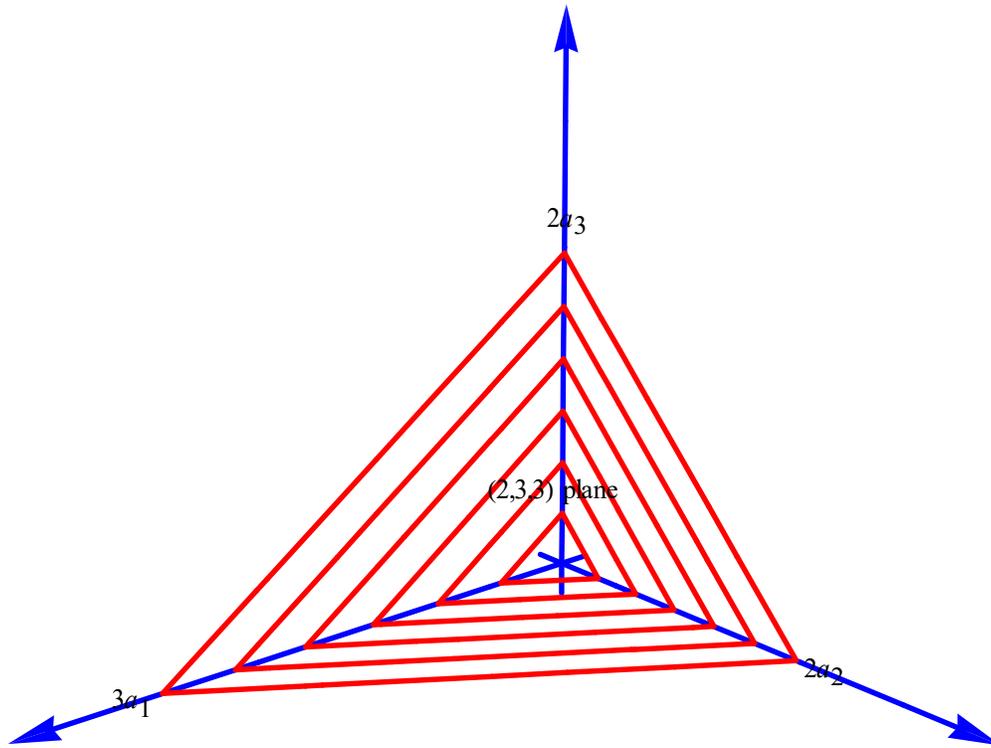


Fig. Planes with the miller indices (233) with $n = 1, 2, 3, 4, 5,$ and 6 . The plane (233) with $n = 6$ intersects at $3a_1, 2a_2, 2a_3$.

23. Example

We consider the plane intercepts the a_1, a_2, a_3 axes at $4a_1, (-1a_2), 2a_3$.

$$\frac{n}{h} = 4, \quad \frac{n}{k} = -1, \quad \frac{n}{l} = 2$$

or

$$h = \frac{n}{4}, \quad k = -n, \quad l = \frac{n}{2}$$

Note that h, k, l and n are integers. When $n = 4$, we have

$$h = 1, \quad k = -4, \quad l = 2.$$

Then we have the plane denoted by $(\bar{1}42)$ with $n = 4$.

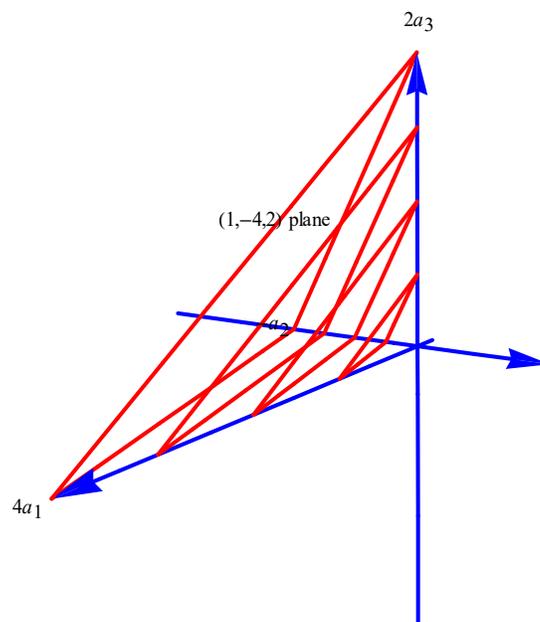


Fig. Planes with the miller indices $(\bar{1}42)$ with $n = 1, 2, 3, 4$. The plane $(\bar{1}42)$ with $n = 4$ intersects at $4a_1, (-1a_2), 2a_3$.

24. (100) plane

We consider the (100) plane. From the definition, we have

- (i) Intercept $a_1 \rightarrow 1 \times (a_1/1) \rightarrow (100)$ plane with $n = 1$
- (ii) Intercept $2a_1 \rightarrow 2 \times (a_1/1) \rightarrow (100)$ plane with $n = 2$
- (iii) Intercept $3a_1 \rightarrow 3 \times (a_1/1) \rightarrow (100)$ plane with $n = 3$

25. (200) plane

We consider the (200) plane.

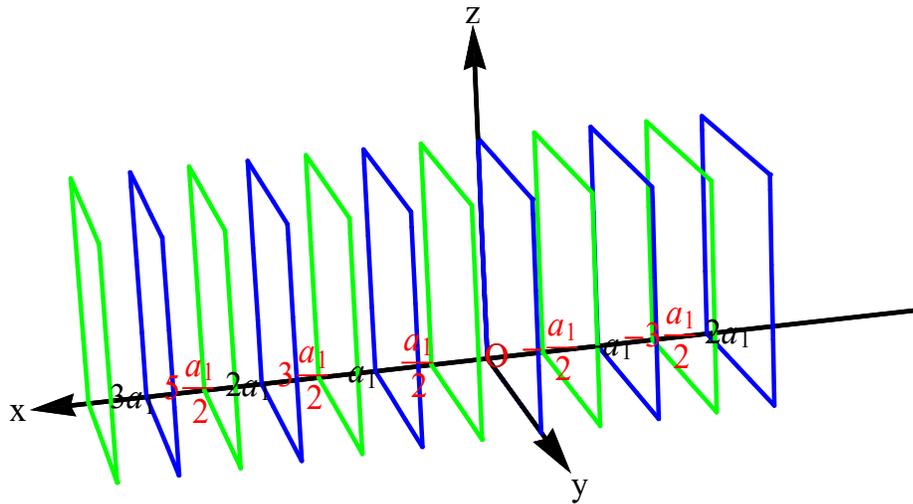


Fig. The family of (100) plane and the family of (200) plane.

- (i) Intercept $a_1/2 \rightarrow 1 \times a_1/2$
(200) plane with $n = 1$
- (ii) Intercept $a_1 \rightarrow 2 \times a_1/2$ [or $1 \times a_1/1$]
(200) plane with $n = 2$ [or (100) plane with $n = 1$]
- (iii) Intercept $3a_1/2 \rightarrow 3 \times a_1/2$
(200) plane with $n = 3$.

- (iv) Intercept $2a_1 \rightarrow 4 \times a_1/2$ [or $2 \times a_1/1$]
 (200) plane with $n = 4$. [or (100) plane with $n = 2$]
- (iv) Intercept $5a_1/2 \rightarrow 5 \times a_1/2$
 (200) plane with $n = 5$.

26. Link

Miller indices (Cambridge University)

http://www.doitpoms.ac.uk/tlplib/miller_indices/index.php

Crystal lattice structures

<http://cst-www.nrl.navy.mil/lattice/>

Crystal structures (Wikipedia)

http://en.wikipedia.org/wiki/Crystal_structure

Crystal structures, Rotable 3D models

<http://neubert.net/Crystals/CRYStruc.html>