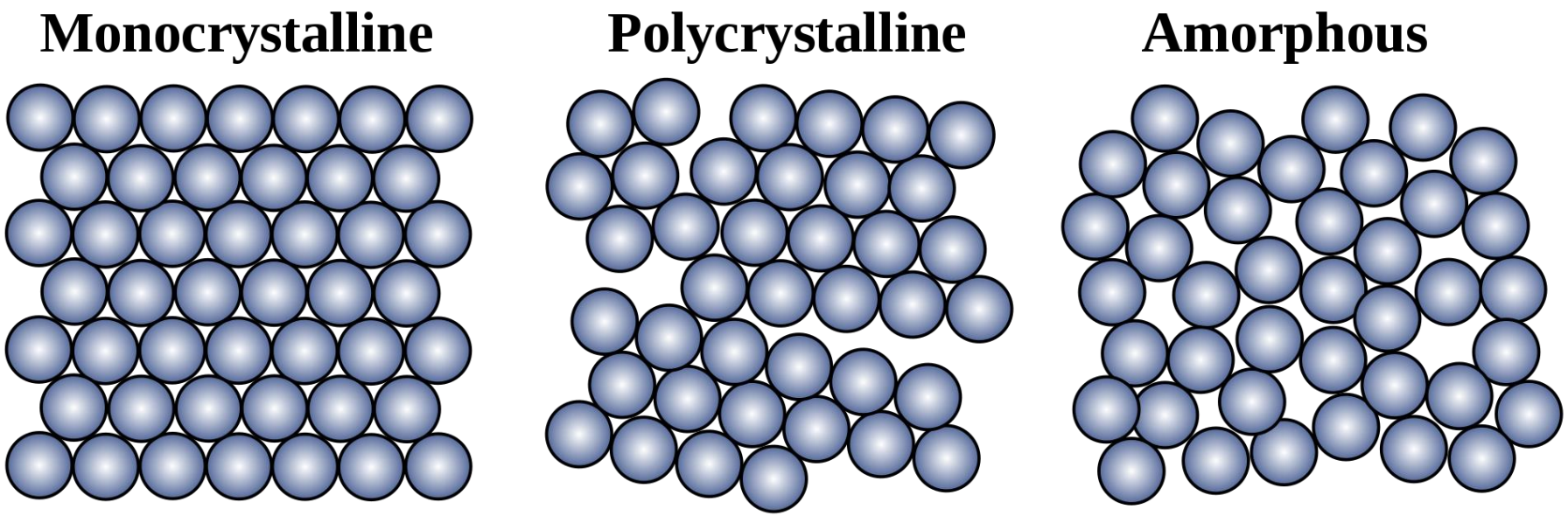
EEE 2105
Electrical Engineering Materials

Elementary Materials Science Concepts

Dr. Mohammad Abdur Rashid

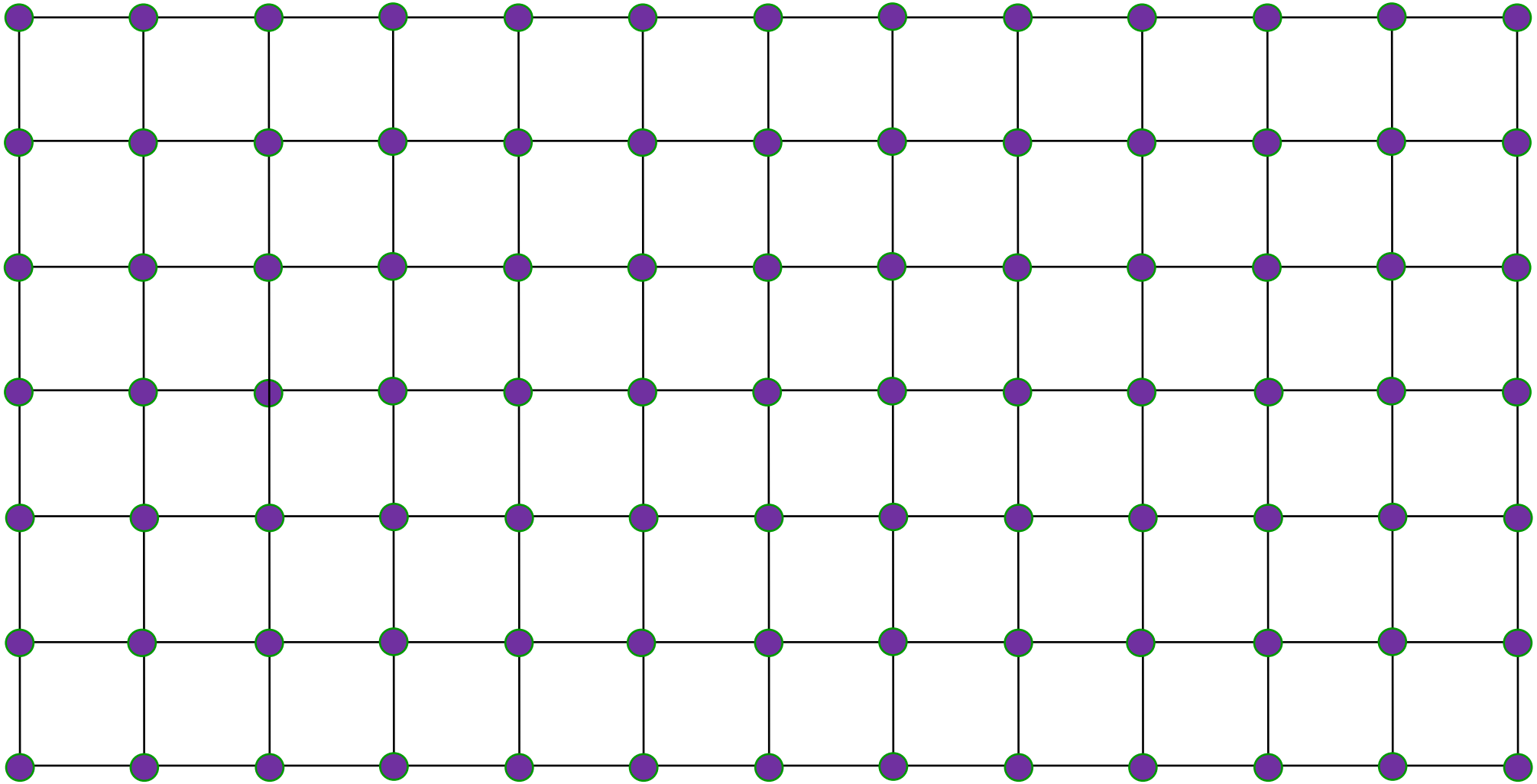
Classification of solids

Solids are broadly classified into two types crystalline solids and amorphous solids.

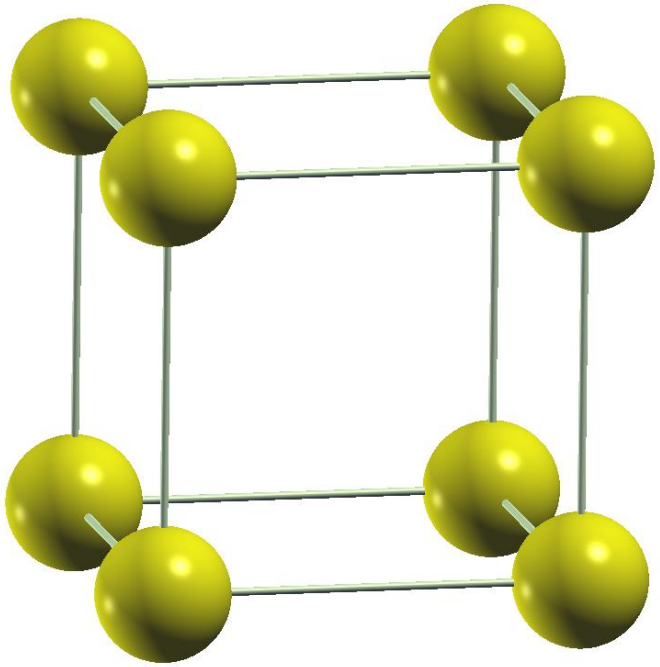


WIKIPEDIA
The Free Encyclopedia

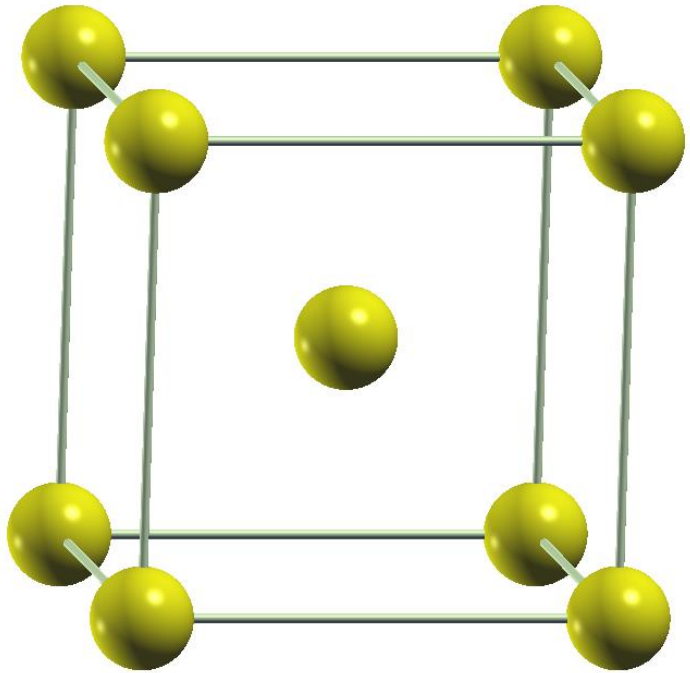
2D Crystal



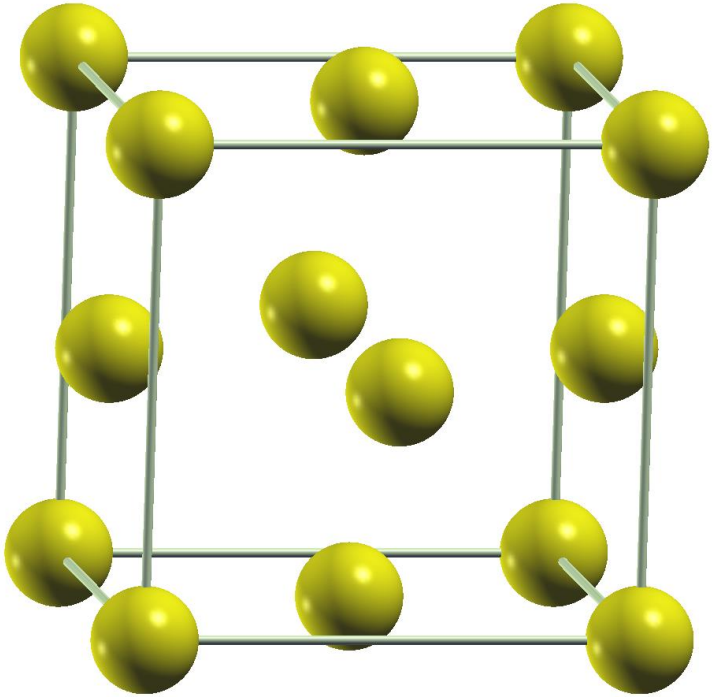
3D Crystal



Simple cubic



Body-centered cubic



Face-centered cubic

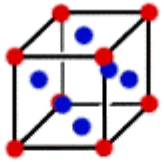
Unit cell

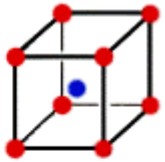
The Simplest Repeating Unit in a Crystal

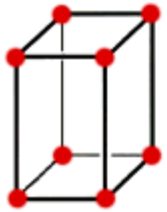
The simplest repeating unit in a crystal is called a **unit cell**. Each unit cell is defined in terms of **lattice points,** the points in space about which the particles are free to vibrate in a crystal.

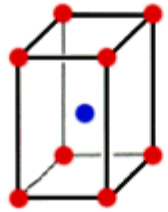
Crystal Systems and Bravais Lattice

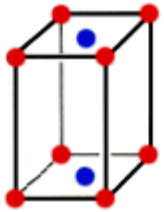

Simple cubic

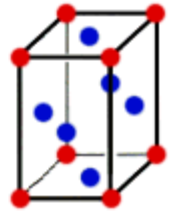

Face-centered cubic

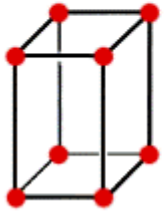

Body-centered cubic

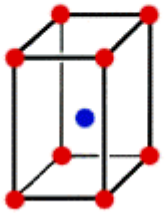

Simple orthorhombic

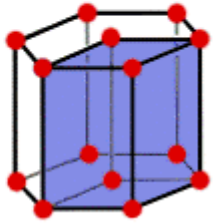

Body-centered orthorhombic


Base-centered orthorhombic

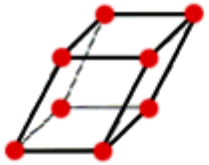

Face-centered orthorhombic

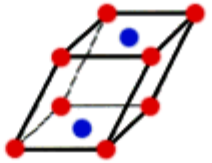

Simple tetragonal

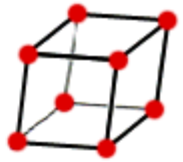

Body-centered tetragonal


Hexagonal


Rhombohedral


Simple Monoclinic


Base-centered monoclinic


Triclinic

epionelynx.wordpress.com

Bravais Lattice

Lattice	Types	Edge Length	Angles between faces	Examples
Cubic	Primitive, Body-centred, Face-centred	$a = b = c$	$\alpha = \beta = \gamma = 90^\circ$	NaCl, Copper and ZnS
Tetragonal	Primitive, Body-centred	$a = b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	White tin, SnO_2, TiO_2 and $CaSO_4$
Orthorhombic	Primitive, Body-centred, Face-centred, End- centred	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	Rhombic Sulphur, $BaSO_4$ and KNO_3
Hexagonal	Primitive	$a = b \neq c$	$\alpha = \beta = 90^\circ$ and $\gamma = 120^\circ$	Graphite, ZnO and CdS
Rhombohedral	Primitive	$a = b = c$	$\alpha = \beta = \gamma \neq 90^\circ$	$CaCO_3$ (Calcite) and HgS (cinnabar)
Monoclinic	Primitive End-centred	$a \neq b \neq c$	$\alpha = \gamma = 90^\circ$ $\beta \neq 90^\circ$	Sulphur
Triclinic	Primitive	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^\circ$	H_3PO_3, $CuSO_4 \cdot 5\ H_2O$

Bravais lattice

A Bravais lattice, studied by Auguste Bravais (1850), is an infinite array of discrete points in three dimensional space generated by a set of discrete translation operations described by:

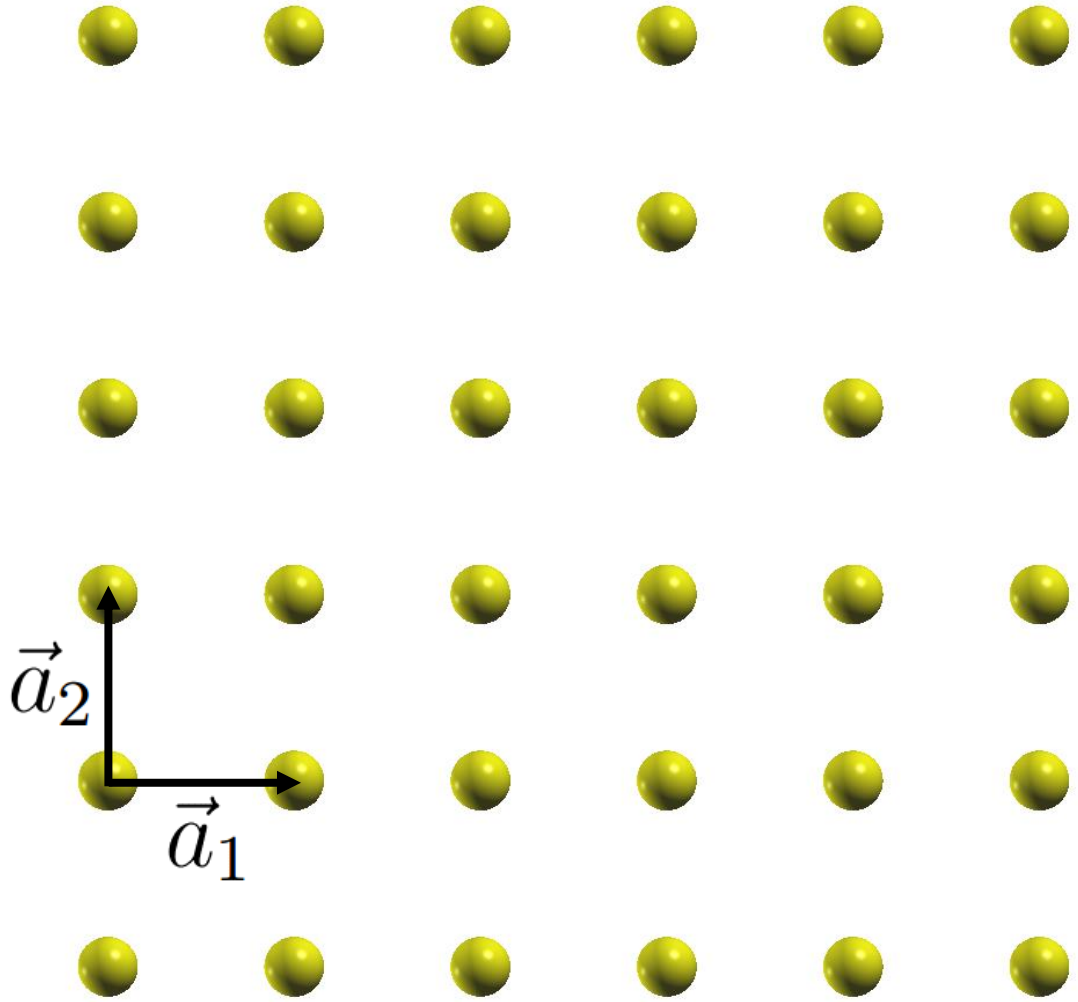
$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$

Where n_i are any integers and $\vec{a}_i$ are known as the primitive vectors which lie in different directions and span the lattice. This discrete set of vectors must be closed under vector addition and subtraction. For any choice of position vector $\vec{R}$, the lattice looks exactly the same.

2D Crystal

$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2$$

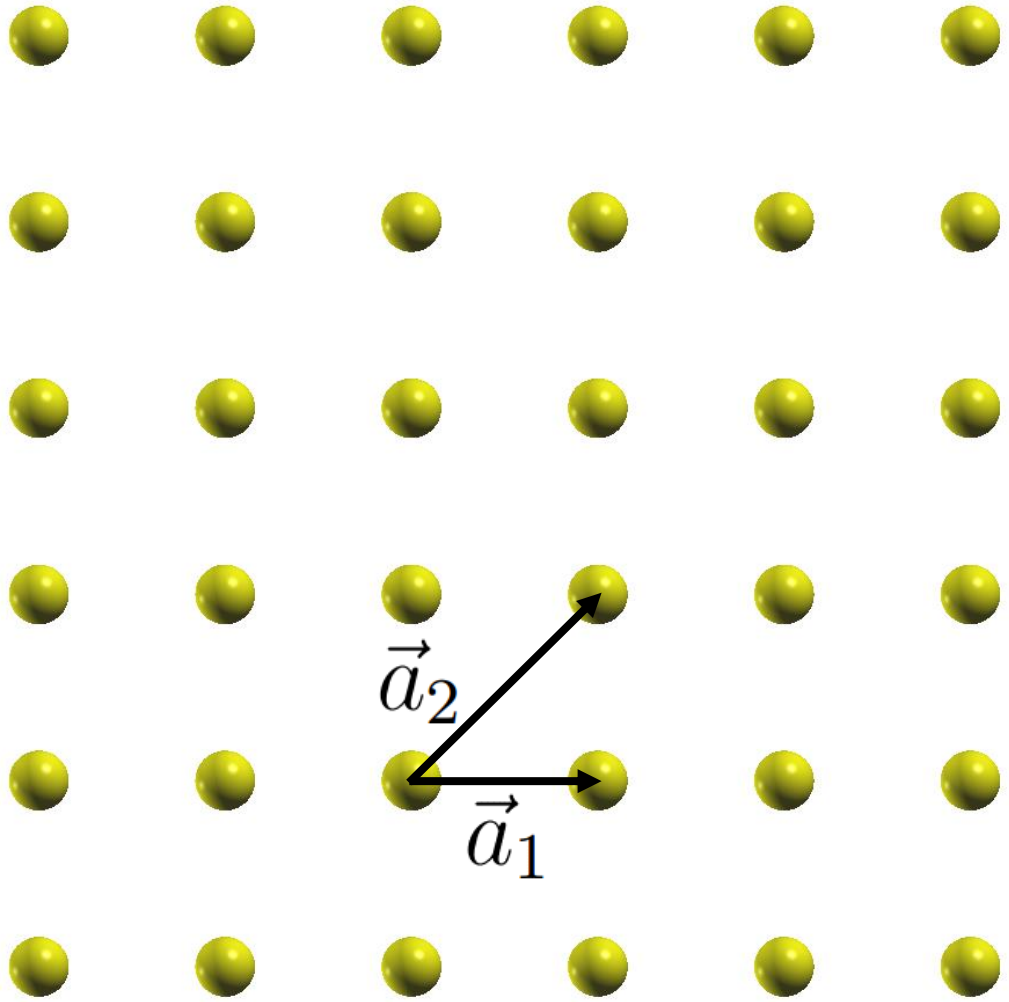
1	0
0	1
1	1
2	2



2D Crystal

$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2$$

1	0
0	1
-1	1
1	1
-2	2



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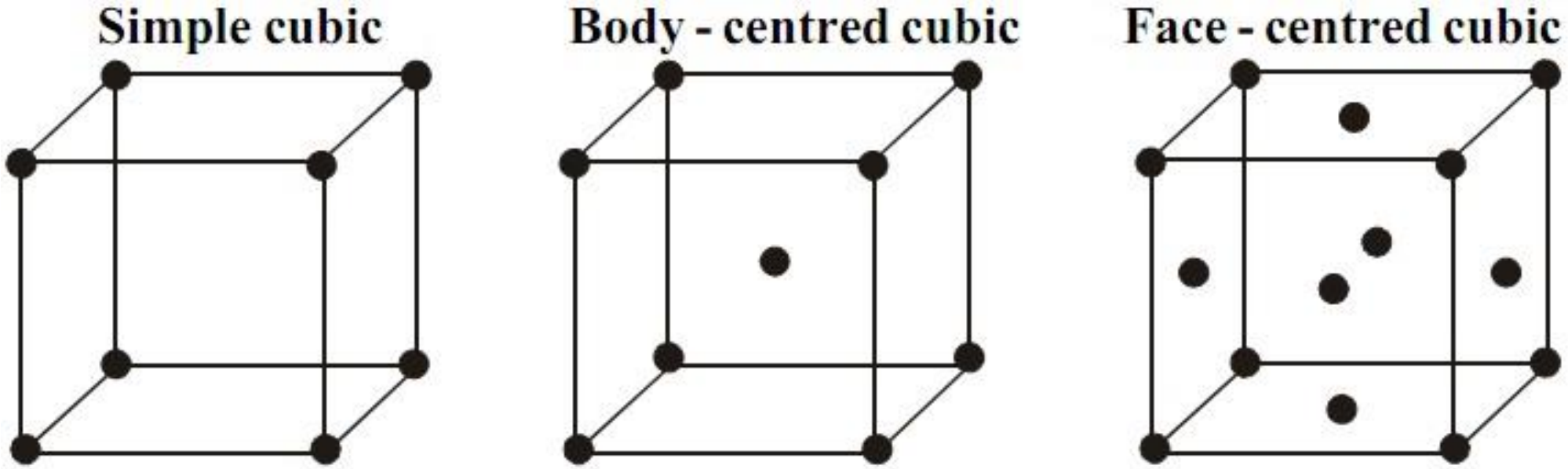
Bravais lattice in 3D



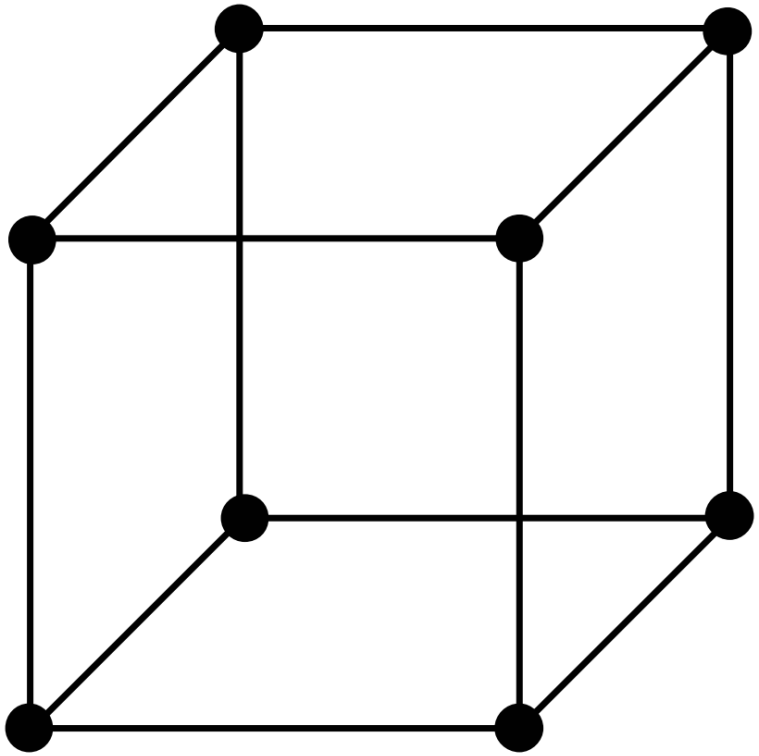
$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$

Primitive lattice vector of sc system

$$\vec{a}_1 = a\hat{x}$$

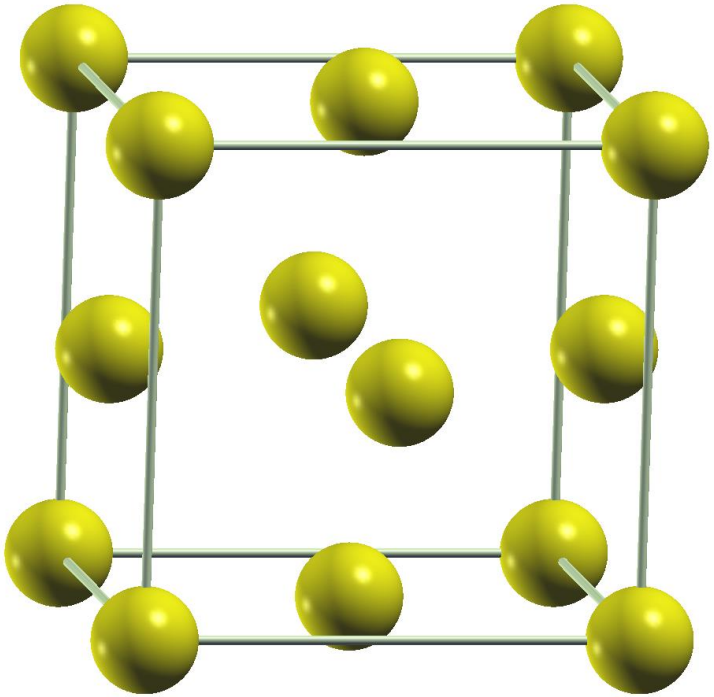
$$\vec{a}_2 = a\hat{y}$$

$$\vec{a}_3 = a\hat{z}$$



$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$

Primitive lattice vector of fcc system



$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$

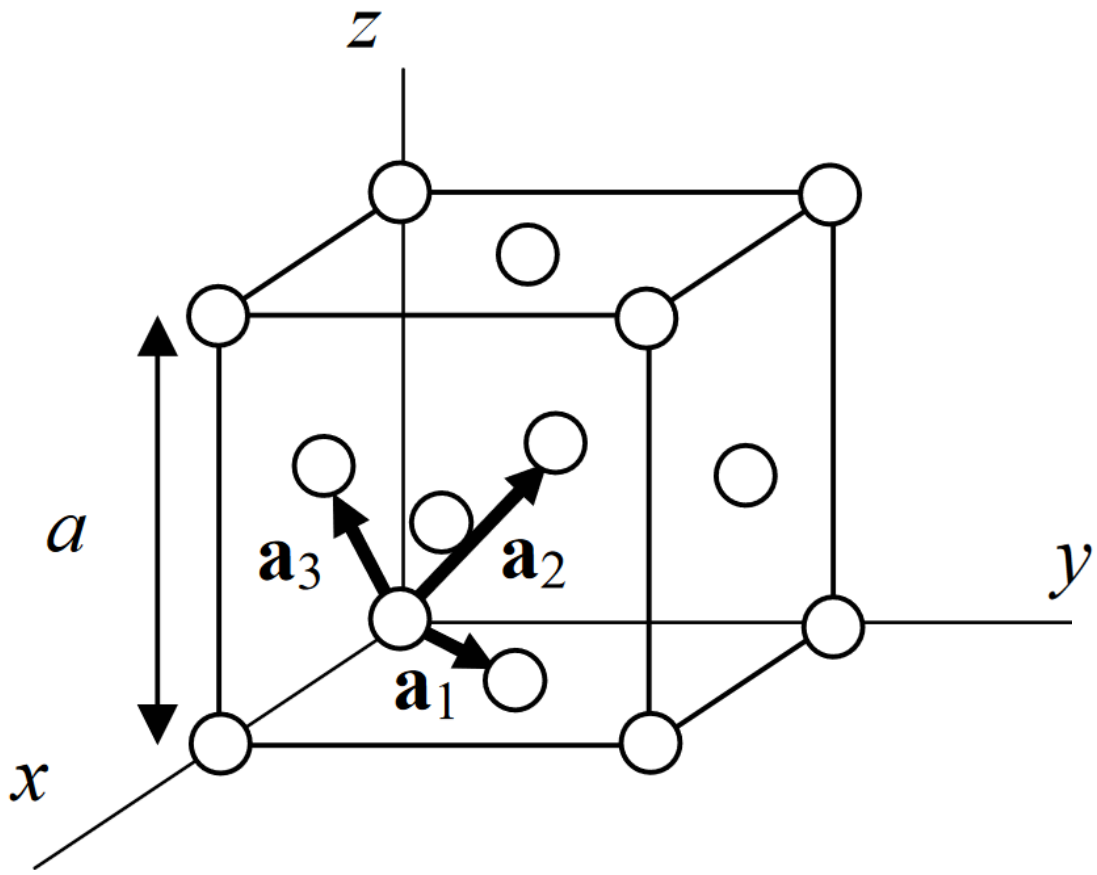
Primitive lattice vector of fcc system

$$\vec{a}_1 = \frac{a}{2}(\hat{x} + \hat{y})$$

$$\vec{a}_2 = \frac{a}{2}(\hat{y} + \hat{z})$$

$$\vec{a}_3 = \frac{a}{2}(\hat{z} + \hat{x})$$

$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$



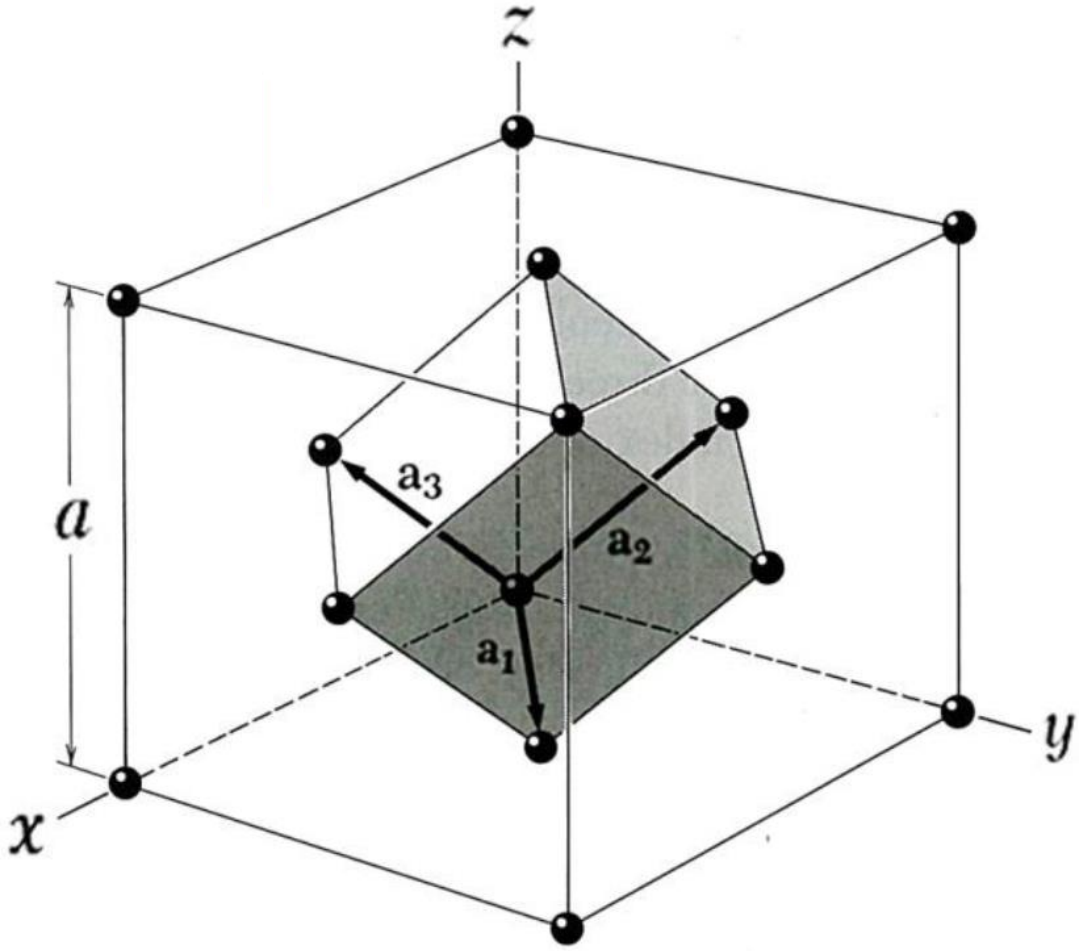
Primitive lattice vector of fcc system

$$\vec{a}_1 = \frac{a}{2}(\hat{x} + \hat{y})$$

$$\vec{a}_2 = \frac{a}{2}(\hat{y} + \hat{z})$$

$$\vec{a}_3 = \frac{a}{2}(\hat{z} + \hat{x})$$

$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$



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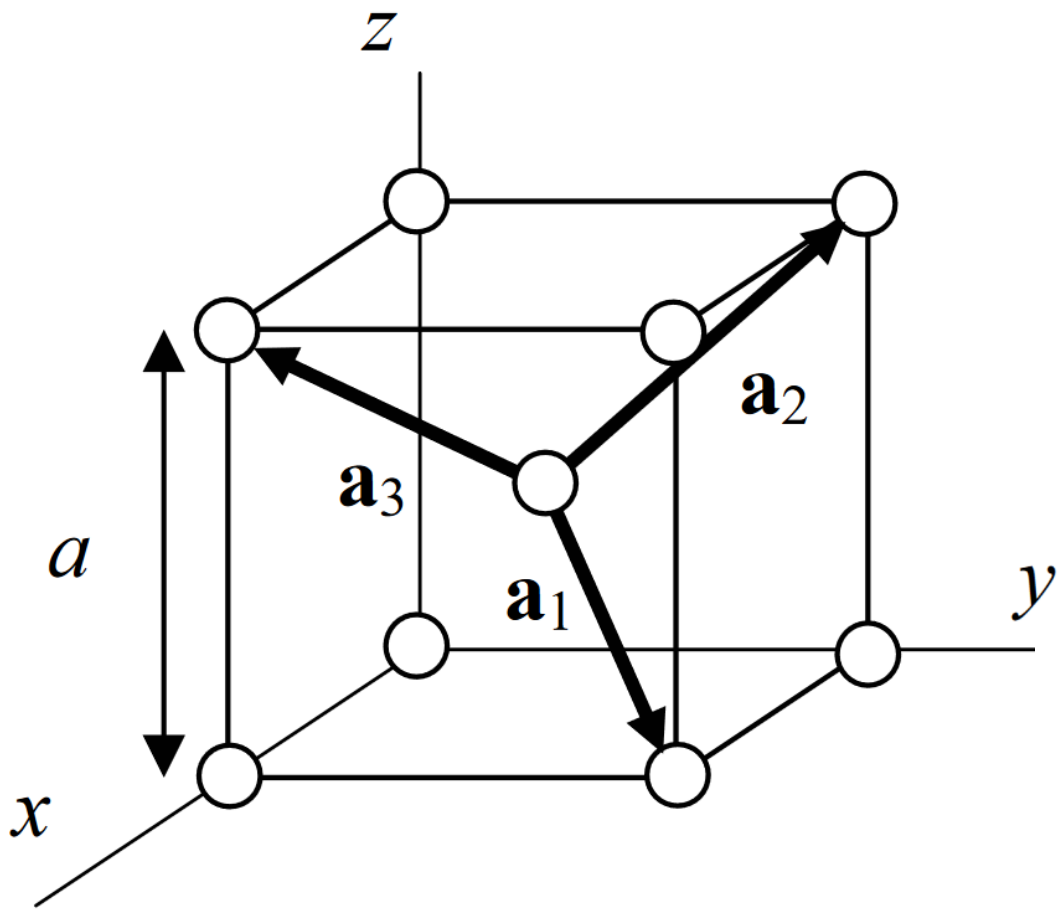
Primitive lattice vector of bcc system

$$\vec{a}_1 = \frac{a}{2}(\hat{x} + \hat{y} - \hat{z})$$

$$\vec{a}_2 = \frac{a}{2}(\hat{y} + \hat{z} - \hat{x})$$

$$\vec{a}_3 = \frac{a}{2}(\hat{z} + \hat{x} - \hat{y})$$

$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$



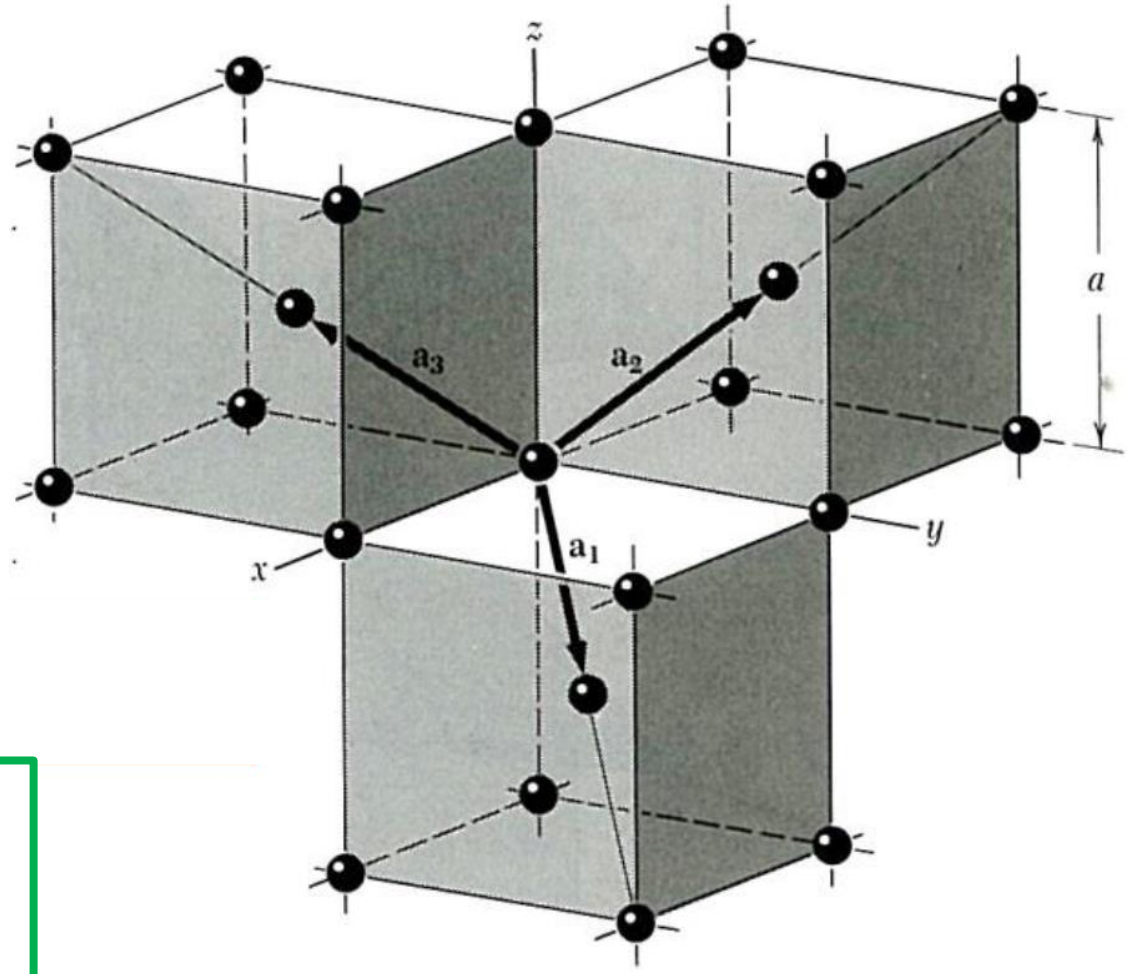
Primitive lattice vector of bcc system

$$\vec{a}_1 = \frac{a}{2}(\hat{x} + \hat{y} - \hat{z})$$

$$\vec{a}_2 = \frac{a}{2}(\hat{y} + \hat{z} - \hat{x})$$

$$\vec{a}_3 = \frac{a}{2}(\hat{z} + \hat{x} - \hat{y})$$

$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$



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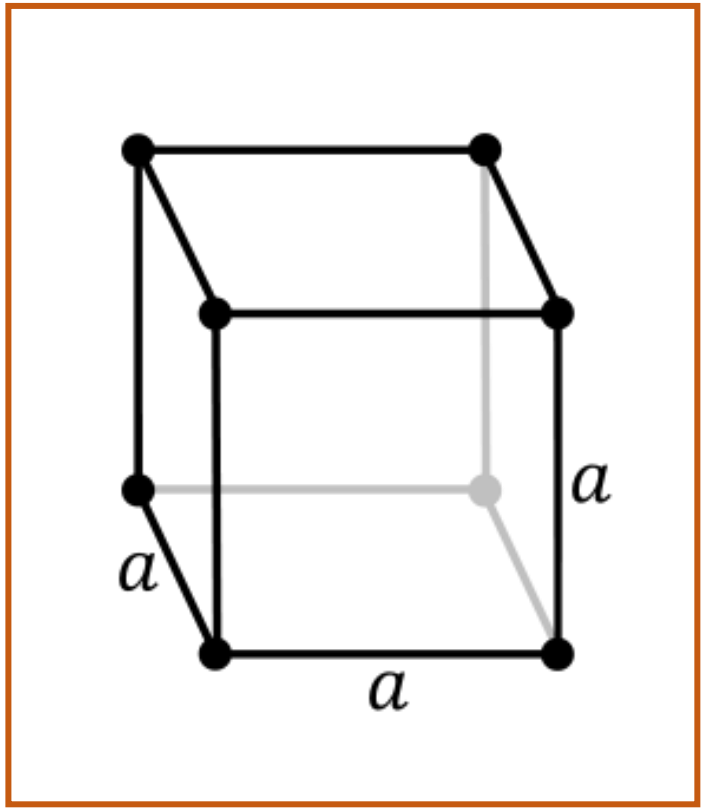
Conventional Unit Cell

A non-primitive unit cell is conventionally chosen for convenience. Typically, these unit cells have a few times the volume of the primitive cell. They can fill space without overlaps and gaps through translational vectors which are sums of multiples of lattice constants. Conventionally, lattice points are assumed to occupy corners of the parallelepiped cells.



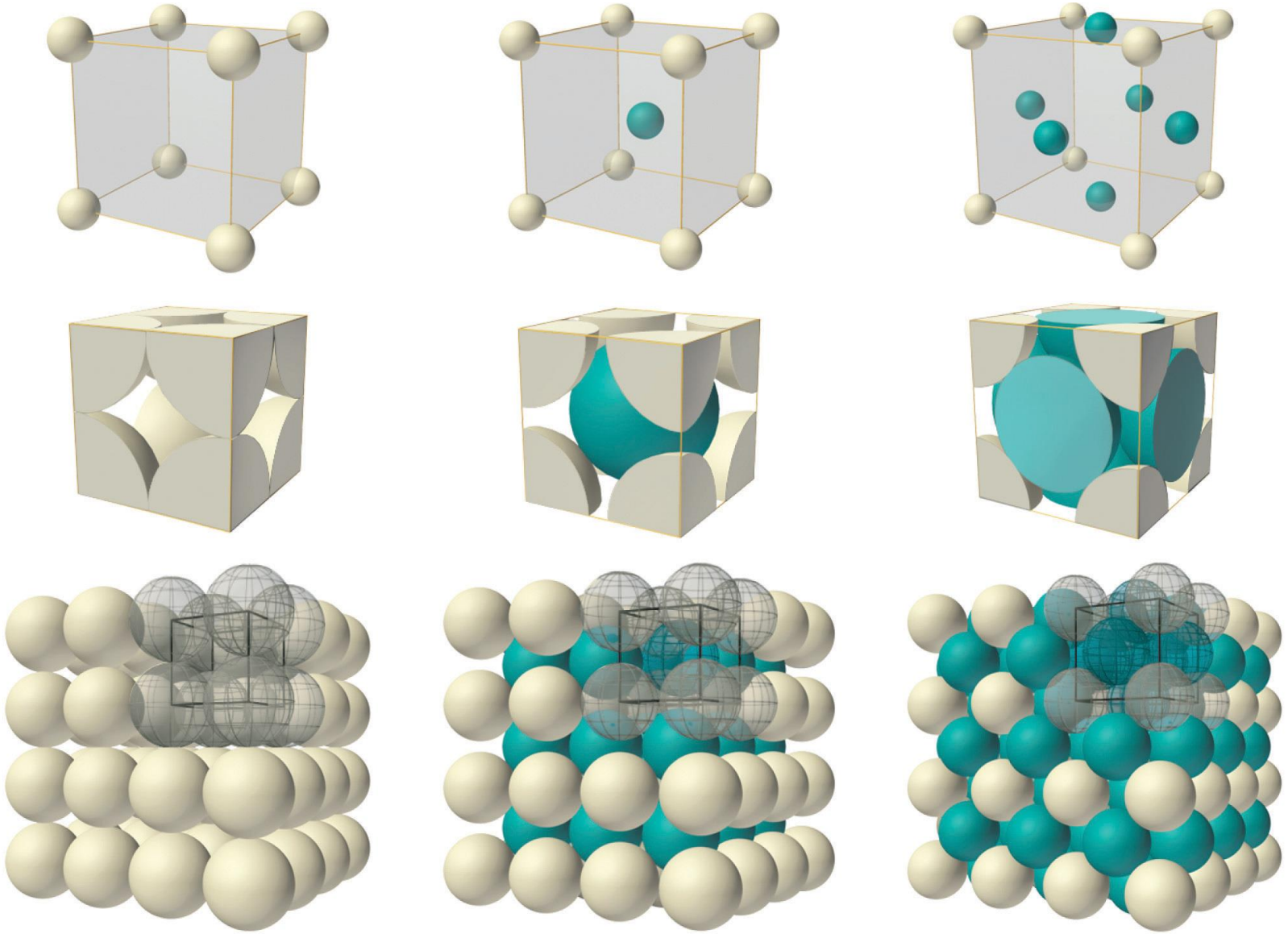
Primitive lattice cell

The parallelepiped defined by primitive axes $\vec{a}_1,\ \vec{a}_2,\ \vec{a}_3$ are called a primitive cell. A primitive cell is a minimum-volume cell. The cell will fill all the space by the repetition of suitable crystal translation operation. There are many ways of choosing the primitive axes and primitive cell for a given lattice.

The volume of a parallelepiped with axes $\vec{a}_1,\ \vec{a}_2,\ \vec{a}_3$ is

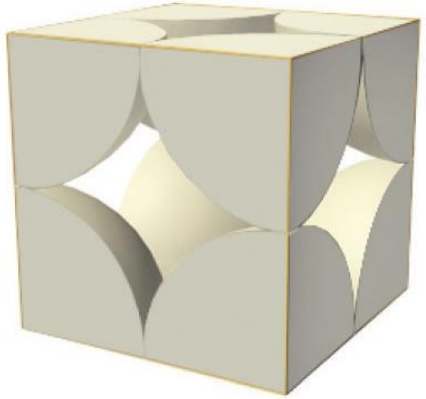
$$V_c = \left|\vec{a}_1 \cdot \left(\vec{a}_2 \times \vec{a}_3\right)\right|$$

3D view showing the number of atoms per unit cell

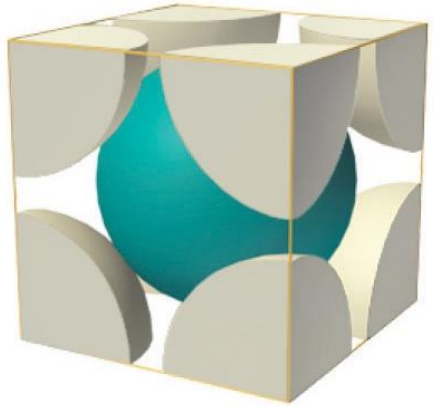


(a) Simple cubic (b) Body-centered cubic (c) Face-centered cubic

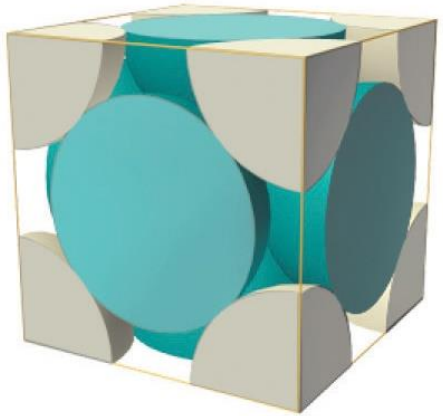
3D view of cubic crystal system



Simple cubic



Body-centered cubic



Face-centered cubic

Atomic packing factor (APF) or packing fraction

Atomic packing factor (APF) or packing fraction is the fraction of volume in a crystal structure that is occupied by constituent particles. It is a dimensionless quantity and always less than unity. In atomic systems, by convention, the APF is determined by assuming that atoms are rigid spheres. The radius of the spheres is taken to be the maximum value such that the atoms do not overlap.

Atomic packing factor (APF) or packing fraction

$$\mathrm{APF} = \frac{N_{\mathrm{particle}} V_{\mathrm{particle}}}{V_{\mathrm{unit\ cell}}}$$

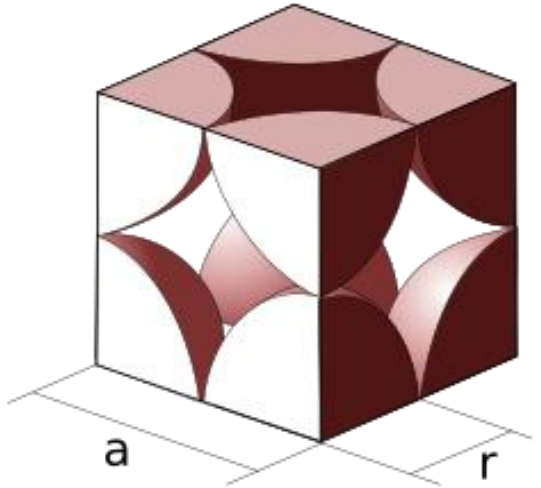
N_{particle} is the number of particles in the unit cell,
V_{particle} is the volume of each particle,
$V_{\mathrm{unit\ cell}}$ is the volume occupied by the unit cell

Atomic packing factor (APF) or packing fraction

Simple cubic

$$\text{APF} = \frac{N_{\text{atoms}} V_{\text{atom}}}{V_{\text{unit cell}}} = \frac{1 \cdot \frac{4}{3}\pi r^3}{(2r)^3}$$

$$= \frac{\pi}{6} \approx 0.5236$$

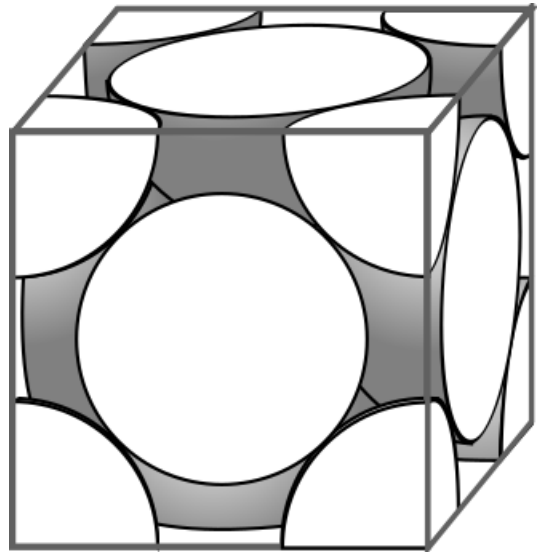


Atomic packing factor (APF) or packing fraction

Face-centered cubic

$$\mathrm{APF} = \frac{N_{\text{atoms}} V_{\text{atom}}}{V_{\text{unit cell}}} = \frac{4 \cdot \frac{4}{3}\pi r^3}{\left(2r\sqrt{2}\right)^3}$$

$$= \frac{\pi\sqrt{2}}{6} \approx 0.740\,48048\,.$$



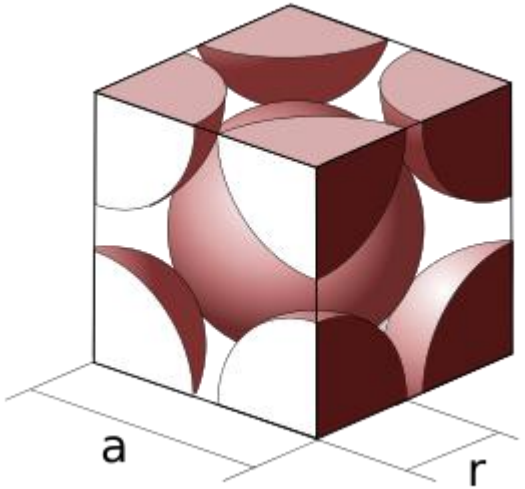
$$a = 2r\sqrt{2}\,.$$

Atomic packing factor (APF) or packing fraction

Body-centered cubic

$$\mathrm{APF} = \frac{N_{\mathrm{atoms}} V_{\mathrm{atom}}}{V_{\mathrm{unit\ cell}}} = \frac{2 \cdot \frac{4}{3}\pi r^3}{\left(\frac{4r}{\sqrt{3}}\right)^3}$$

$$= \frac{\pi\sqrt{3}}{8} \approx 0.680\,174\,762\,.$$

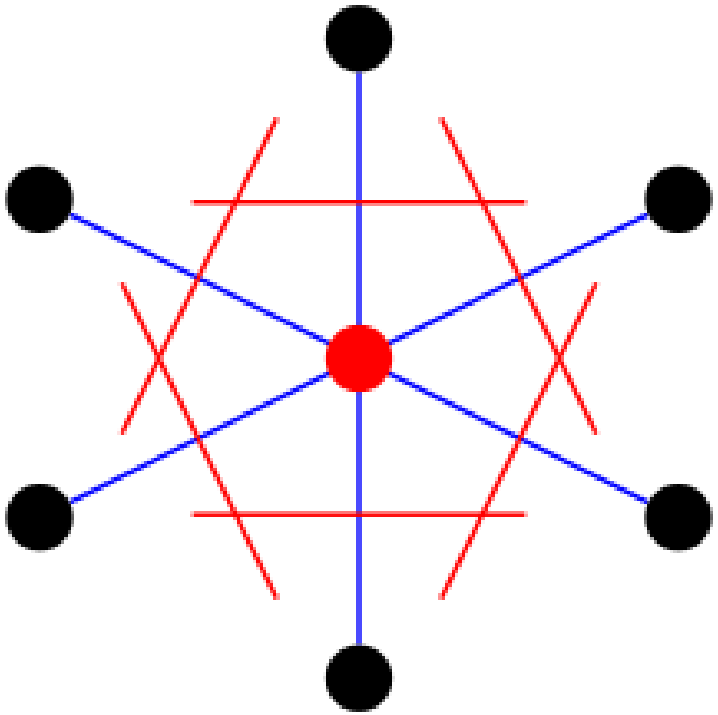


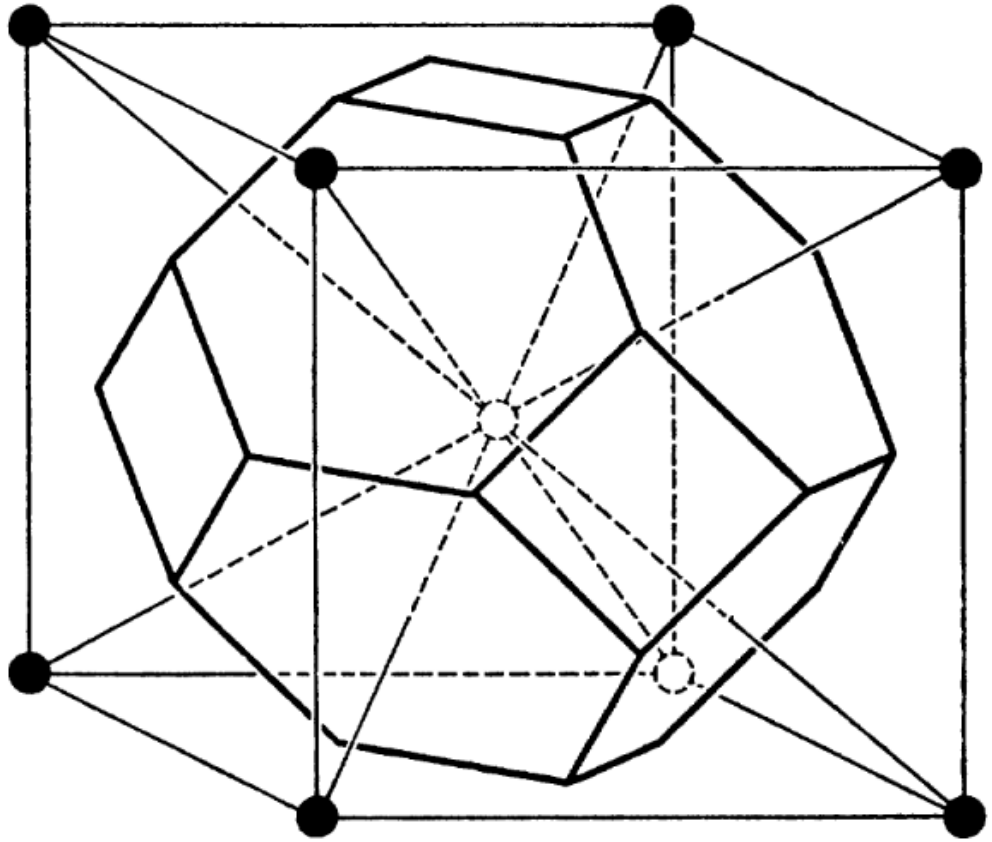
$$a = \frac{4r}{\sqrt{3}}\,.$$

Characteristics of cubic lattices

	Simple	Body-centered	Face-centered
Volume, conventional cell	a^3	a^3	a^3
Lattice points per cell	1	2	4
Volume, primitive cell	a^3	$\frac{1}{2}a^3$	$\frac{1}{4}a^3$
Lattice points per unit volume	$1/a^3$	$2/a^3$	$4/a^3$
Number of nearest neighbors	6	8	12
Nearest-neighbor distance	a	$3^{1/2}\,a/2 = 0.866a$	$a/2^{1/2} = 0.707a$
Number of second neighbors	12	6	6
Second neighbor distance	$2^{1/2}a$	a	a
Packing fraction[a]	$\frac{1}{6}\pi$ $=0.524$	$\frac{1}{8}\pi\sqrt{3}$ $=0.680$	$\frac{1}{6}\pi\sqrt{2}$ $=0.740$

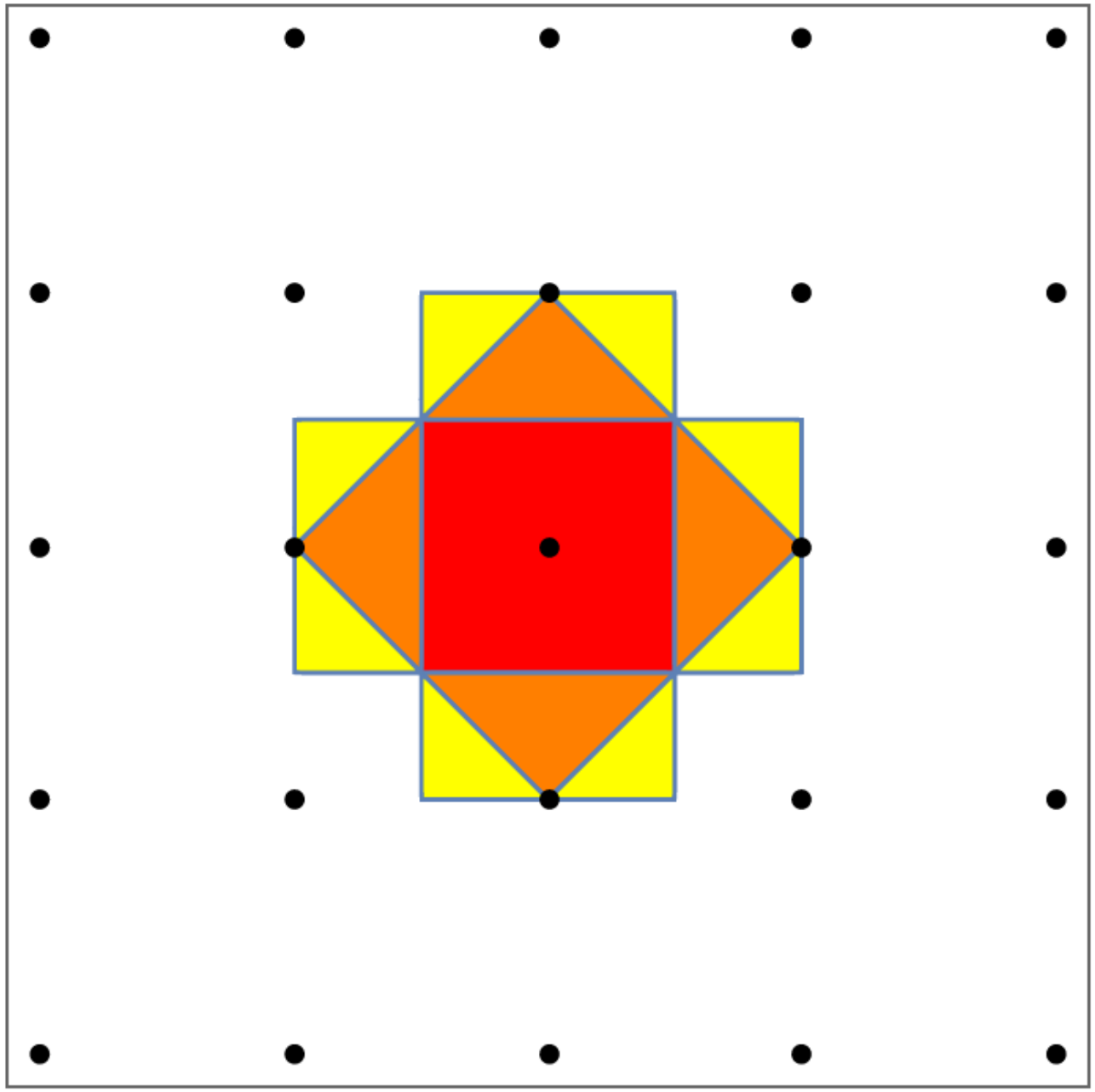
Wigner-Seitz cell





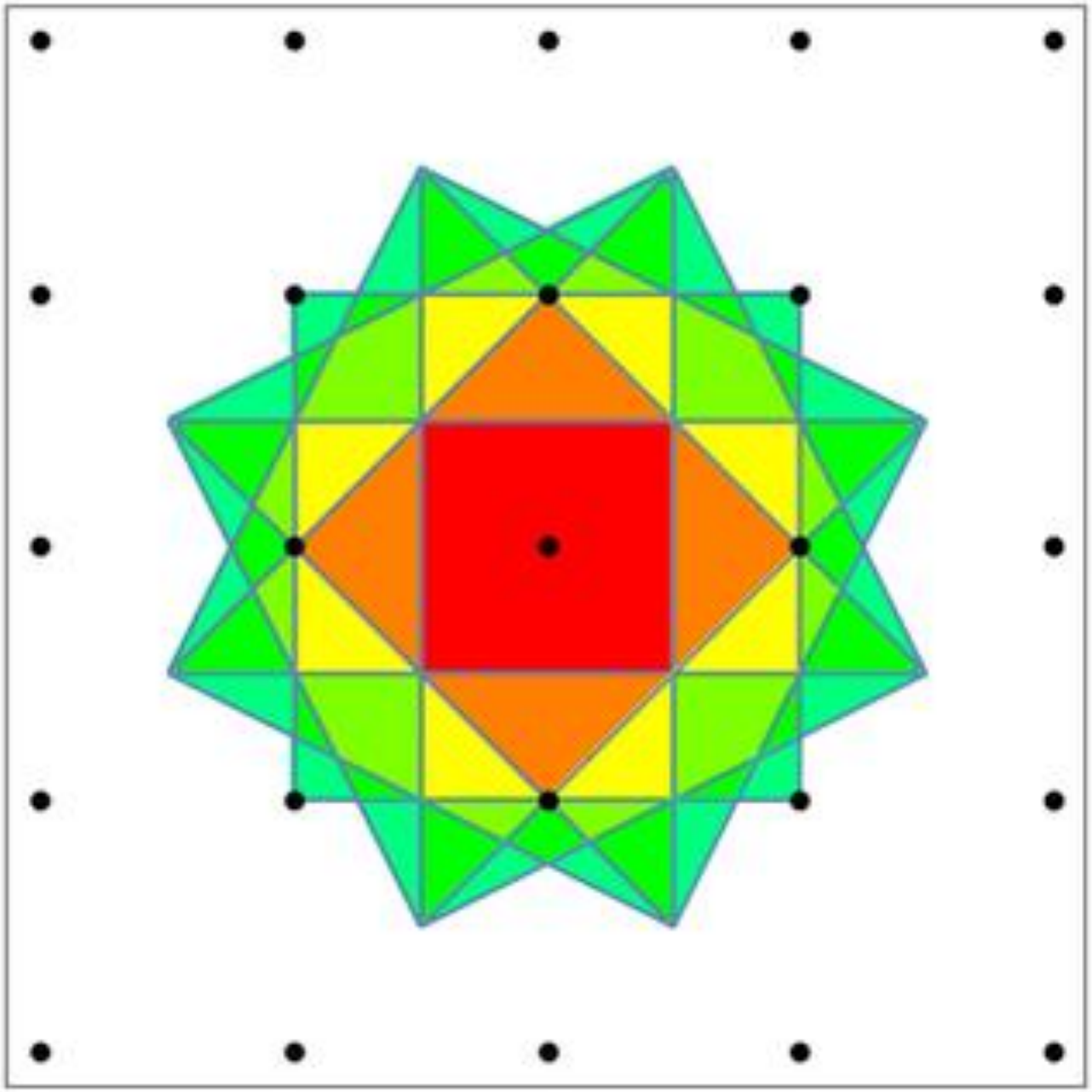
Brillouin zone

https://demonstrations.wolfram.com/2DBrillouinZones/

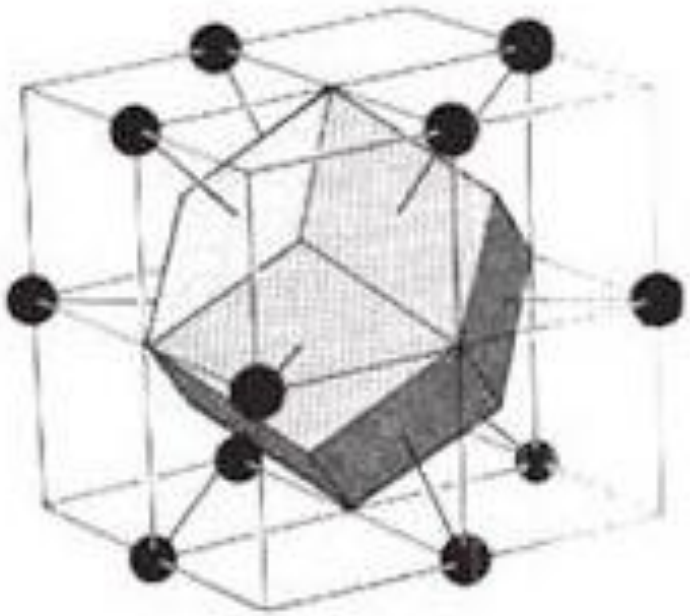


Brillouin zone

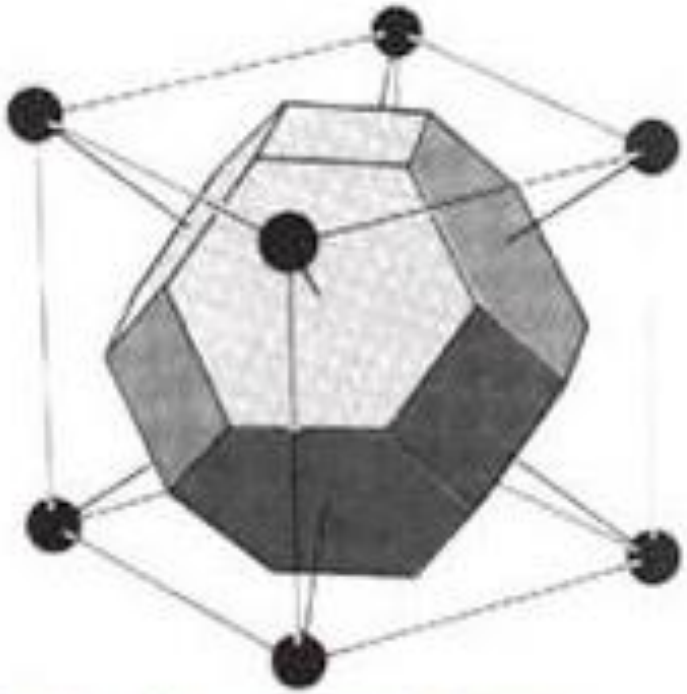
https://demonstrations.wolfram.com/2DBrillouinZones/



Wigner-Seitz cell



Face Centered Cubic
Wigner-Seitz Cell



Body Centered Cubic
Wigner-Seitz Cell

Bravais lattice $\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$

Reciprocal Lattice $\vec{K} = m_1\vec{b}_1 + m_2\vec{b}_2 + m_3\vec{b}_3$

The reciprocal lattice represents the Fourier transform of the Bravais lattice.

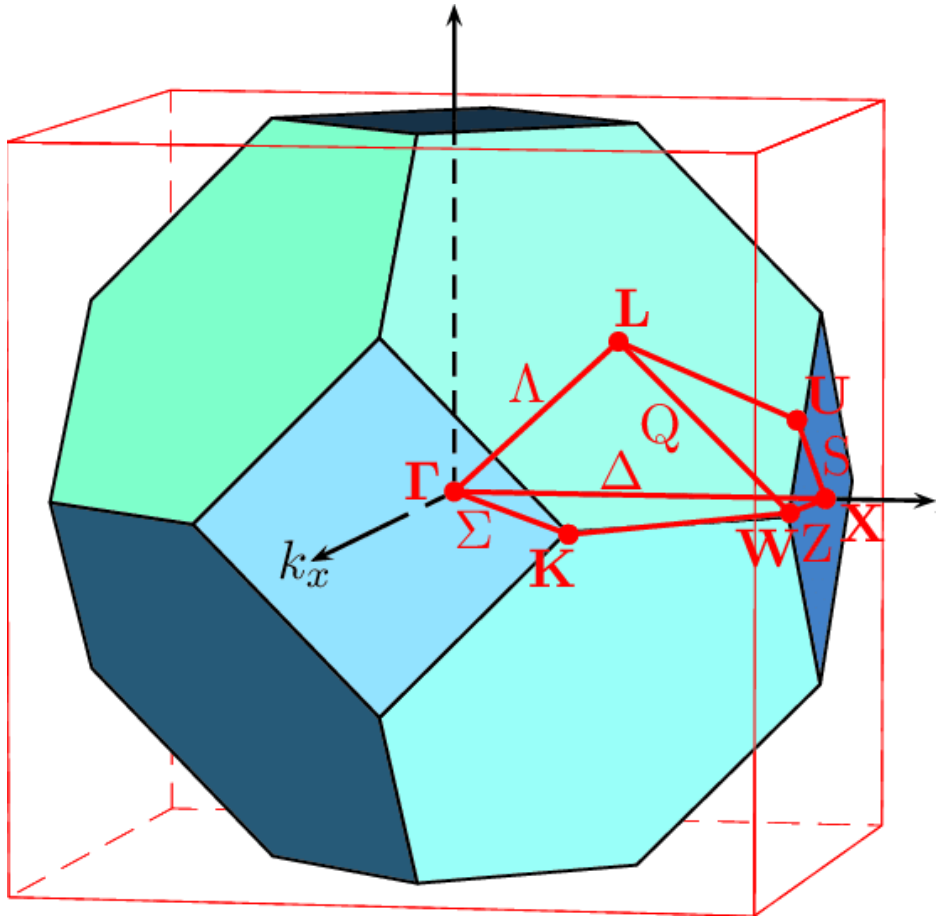
The reciprocal lattice to an fcc lattice is the bcc lattice and vice versa.

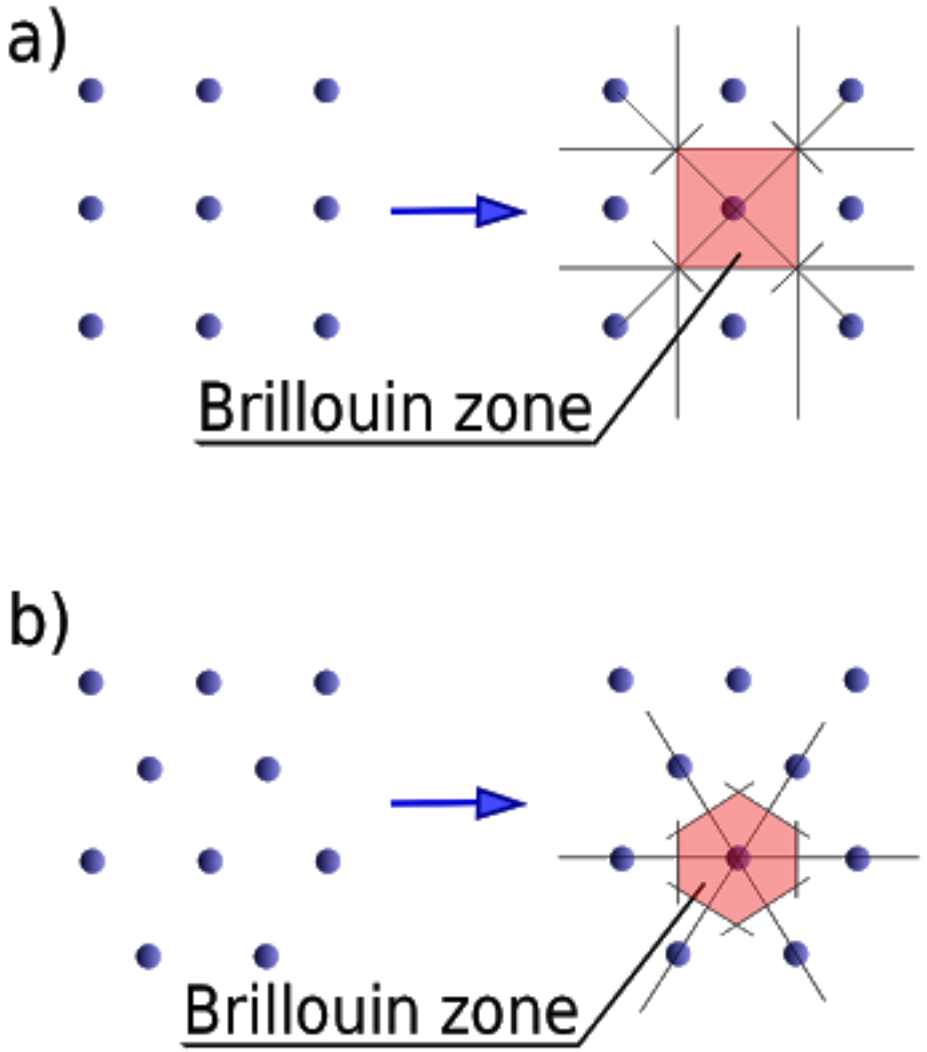
$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_2 \cdot (\vec{a}_3 \times \vec{a}_1)}$$

$$\vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_3 \cdot (\vec{a}_1 \times \vec{a}_2)}$$

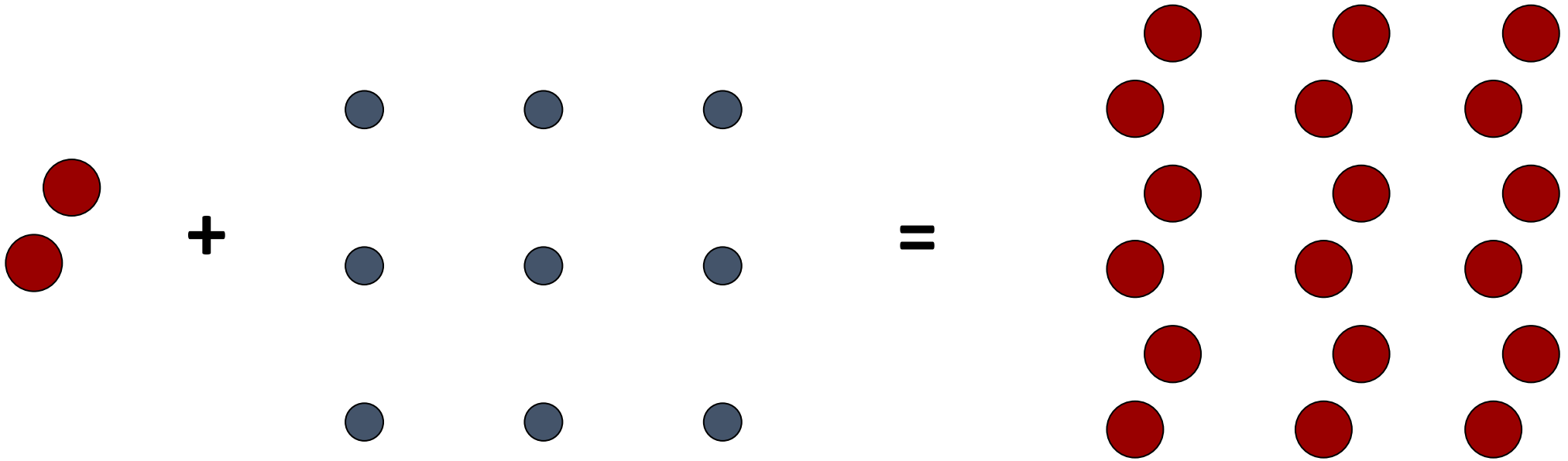
Brillouin zone



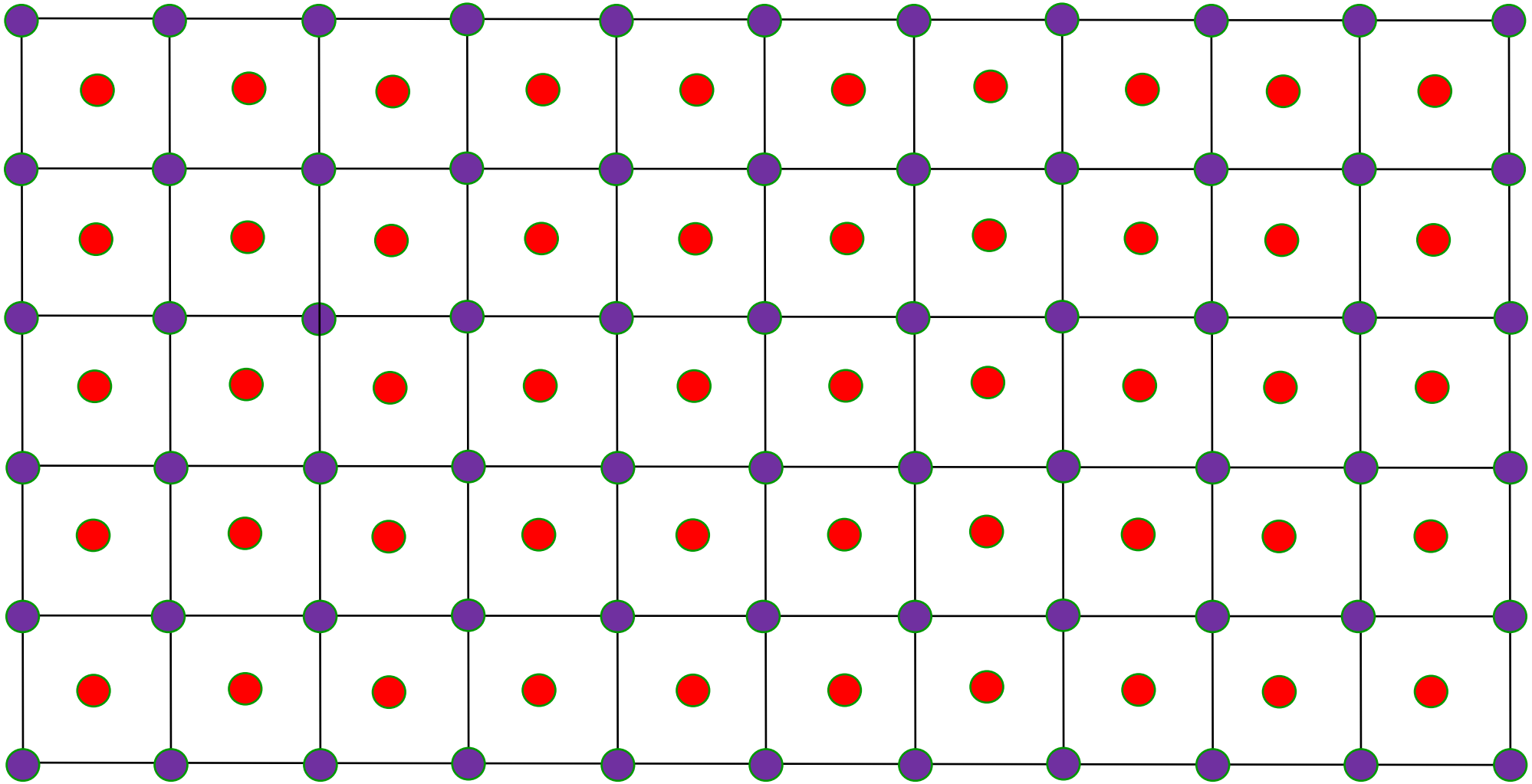


Crystal structure

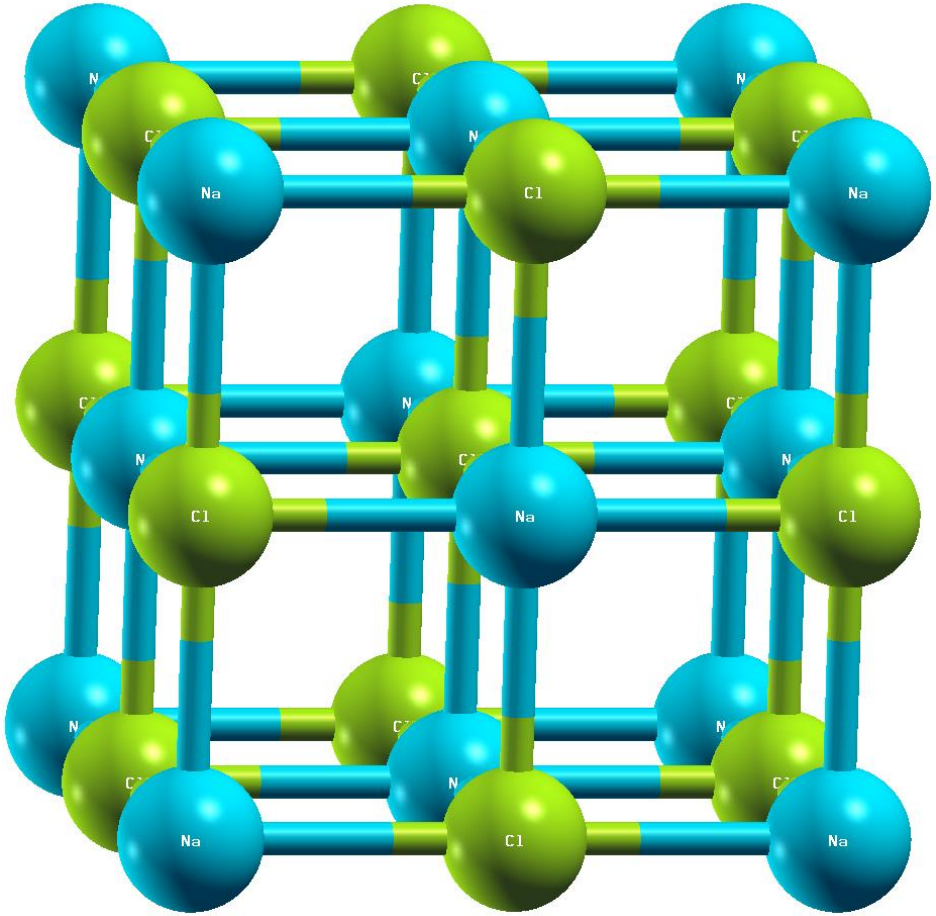
basis + lattice = crystal structure

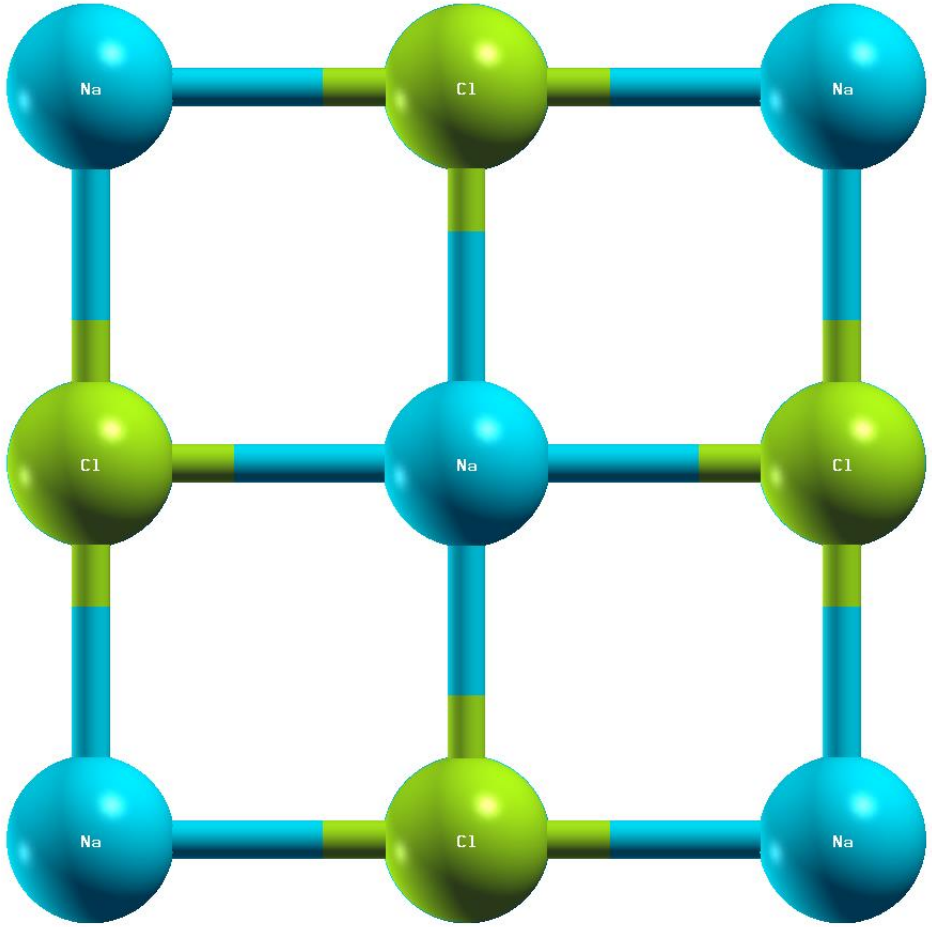


Crystal structure

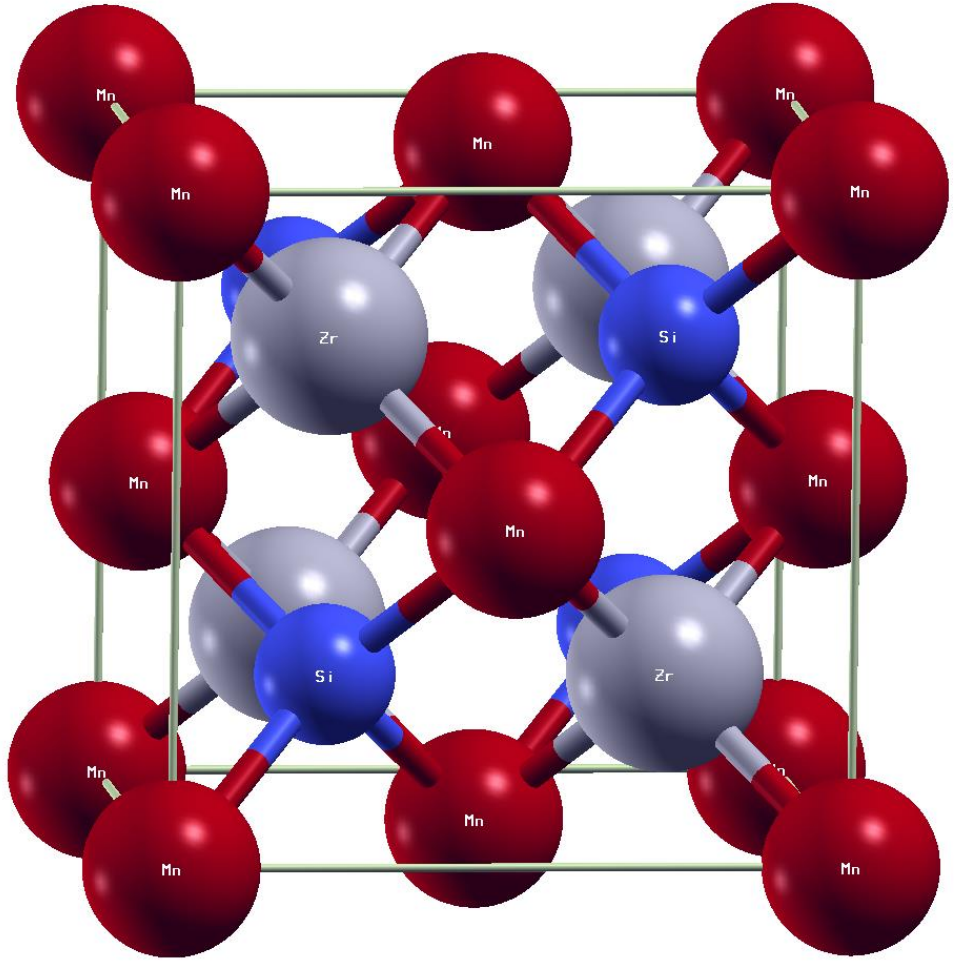


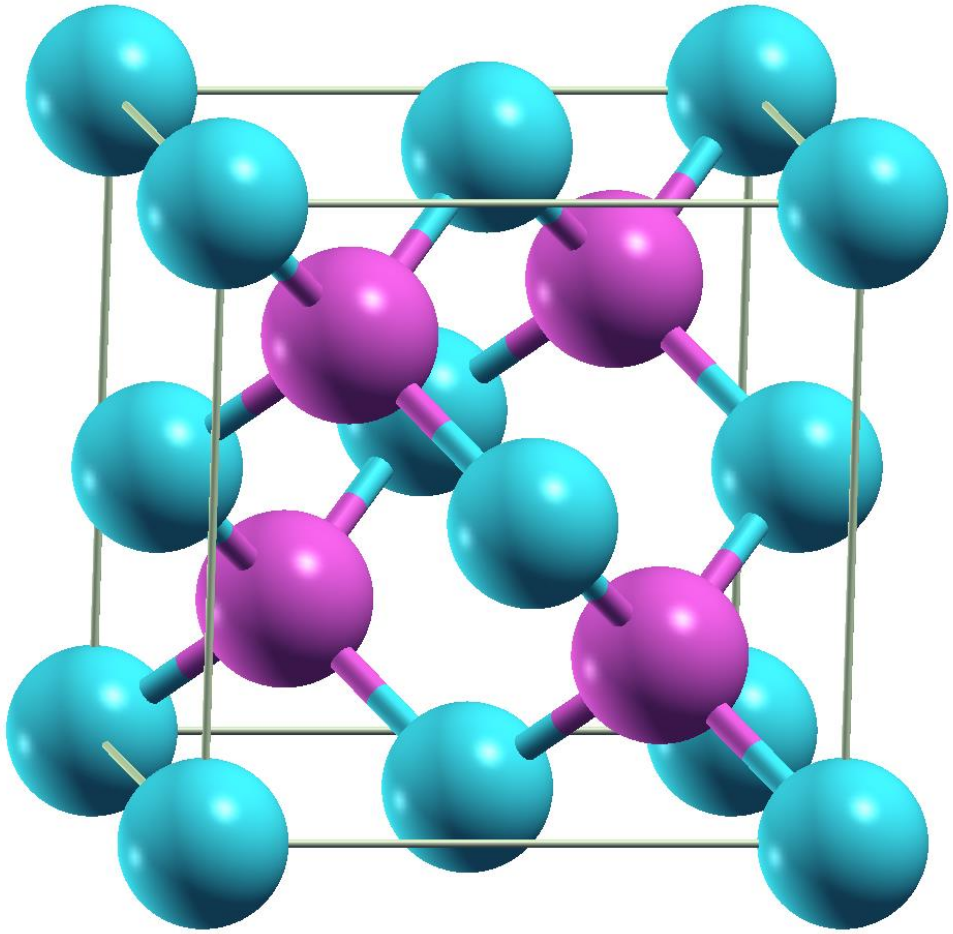
Crystal structure





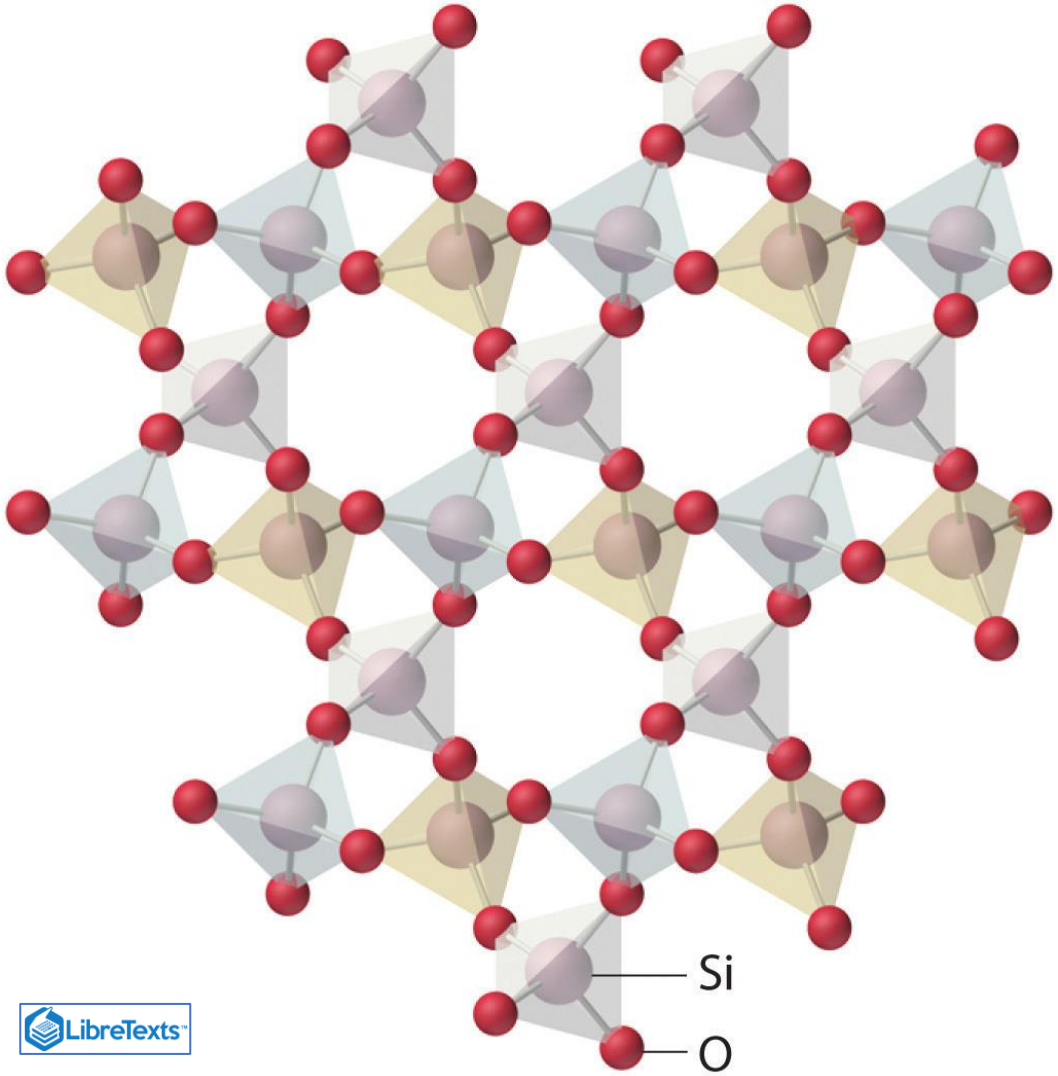
Crystal structure



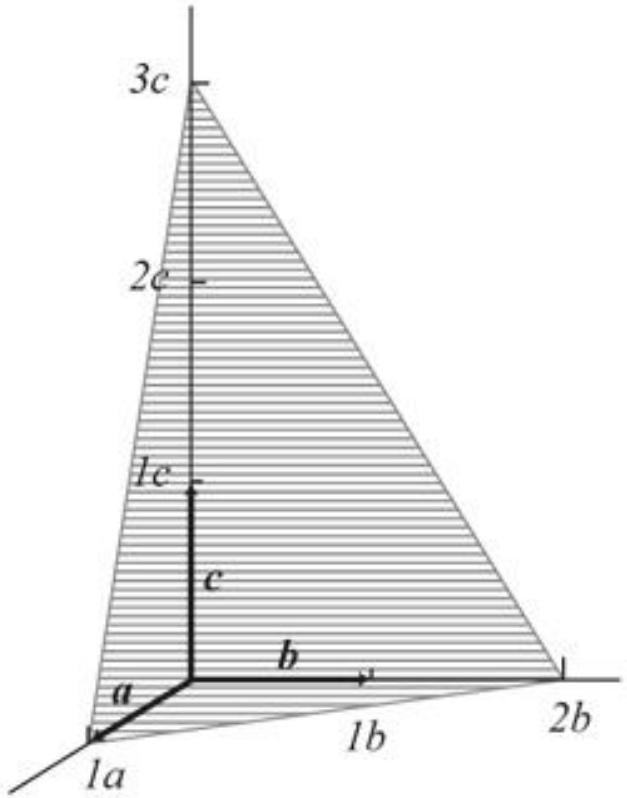


Crystal structure

Crystalline quartz (SiO_2)



Miller Indices



The Miller indices of a lattice plane are the coordinates of the shortest reciprocal lattice vector normal to the plane, with respect to a specific set of primitive reciprocal lattice vectors. Thus a plane with Miller indices ($h\ k\ l$), is normal to the reciprocal lattice vector

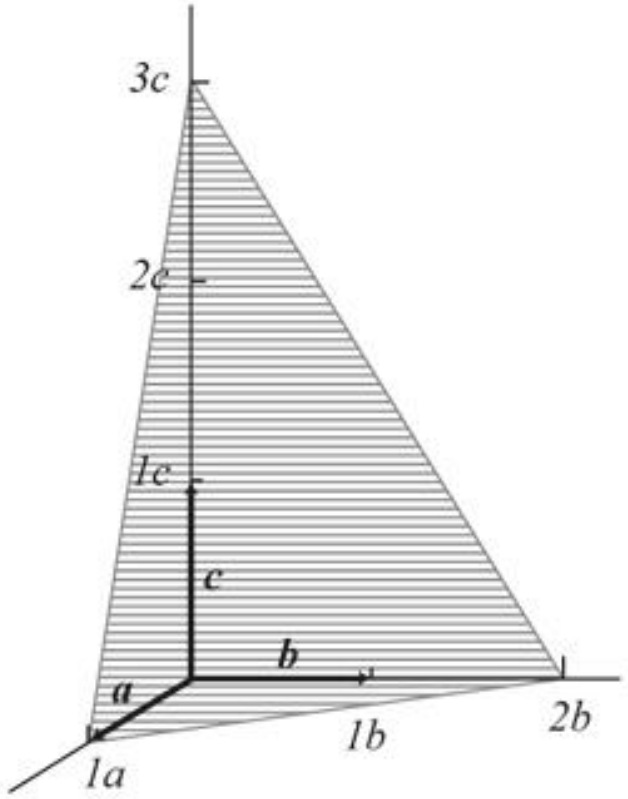
$$h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$$

Miller indices are used to specify directions and planes.

The rules for Miller Indices:

- Determine the intercepts of the face along the crystallographic axes, *in terms of unit cell dimensions.*
- Take the reciprocals
- Clear fractions
- Reduce to lowest terms

$$(1, 2, 3) \rightarrow (\frac{1}{1} : \frac{1}{2} : \frac{1}{3}) \rightarrow (6 : 3 : 2) \rightarrow (632)$$



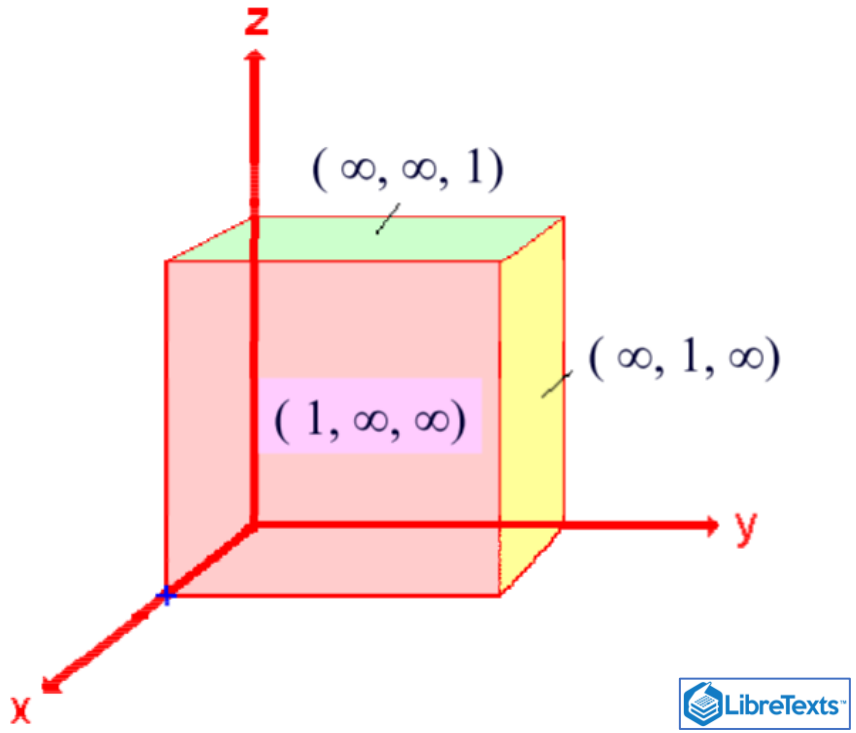
Miller Indices

Miller Indices are the reciprocals of the parameters of each crystal face.

For Pink Face: $\left(\frac{1}{1}, \frac{1}{\infty}, \frac{1}{\infty}\right) \rightarrow (100)$

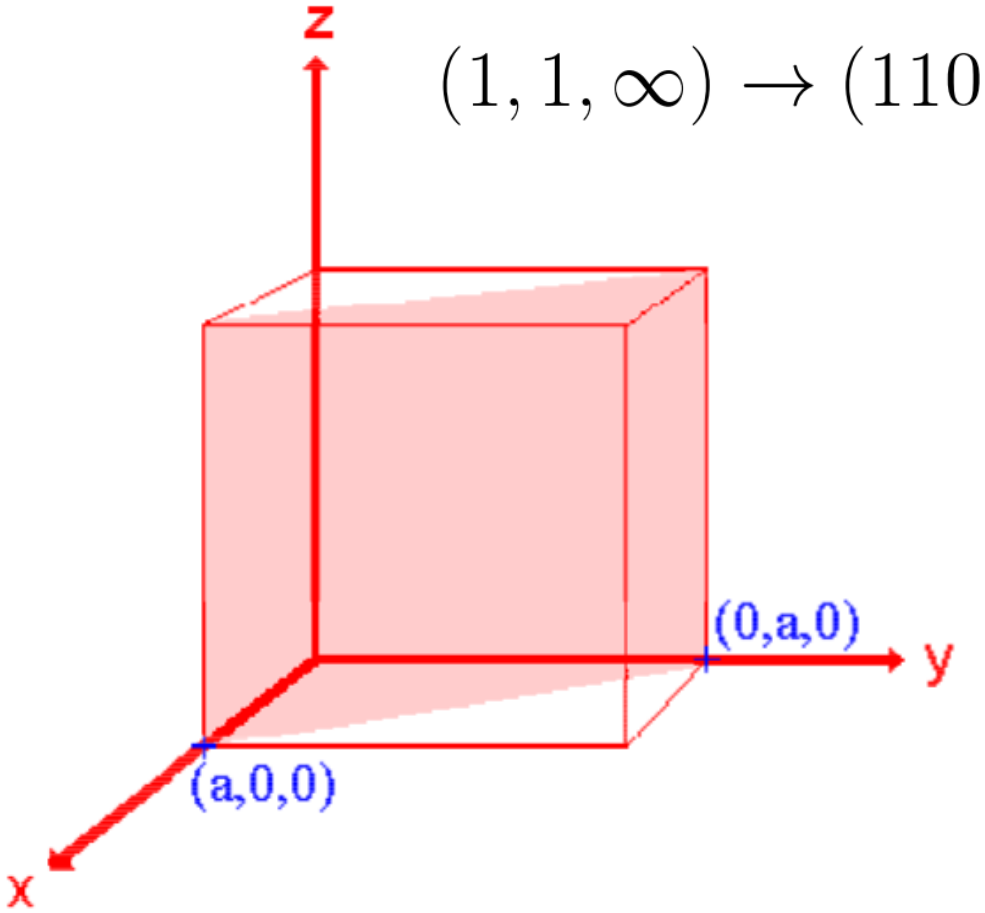
For Green Face: $\left(\frac{1}{\infty}, \frac{1}{\infty}, \frac{1}{1}\right) \rightarrow (001)$

For Yellow Face: $\left(\frac{1}{\infty}, \frac{1}{1}, \frac{1}{\infty}\right) \rightarrow (010)$

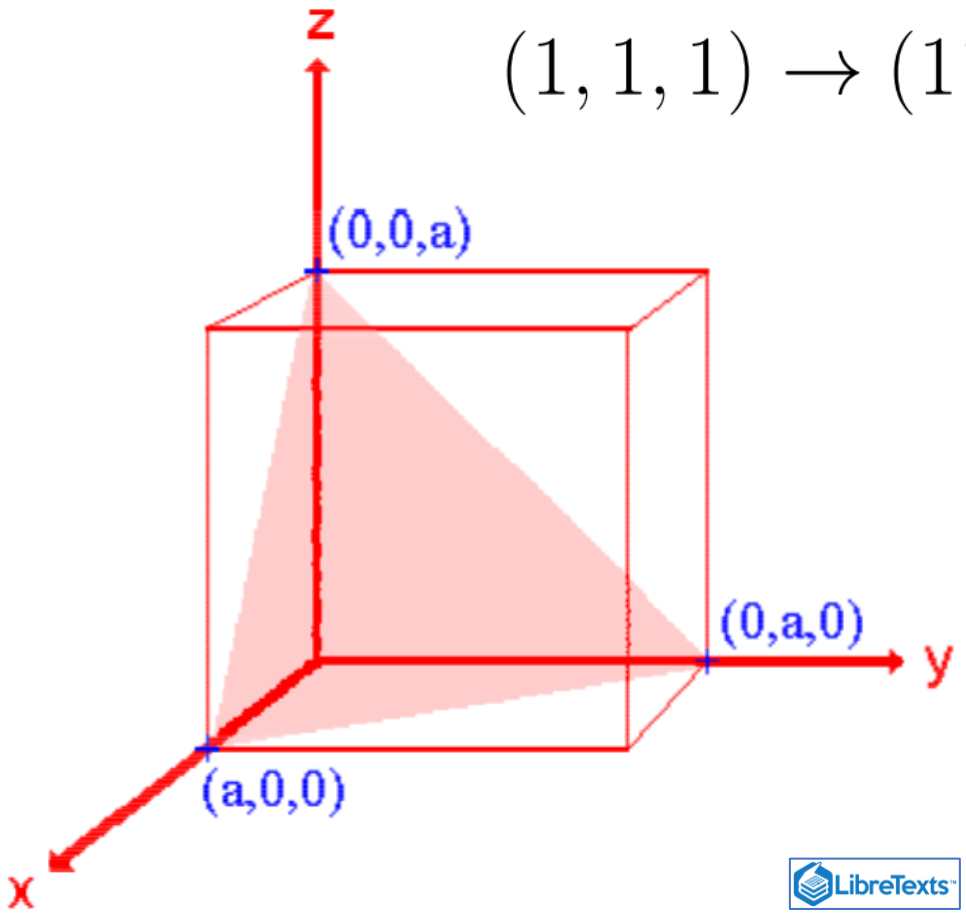


Miller Indices

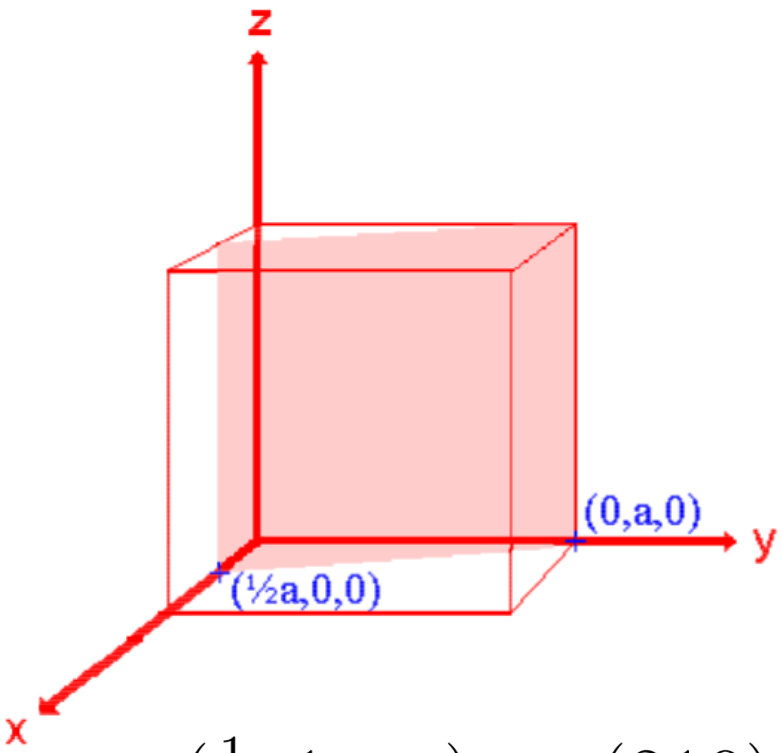
$(1, 1, \infty) \rightarrow (110)$



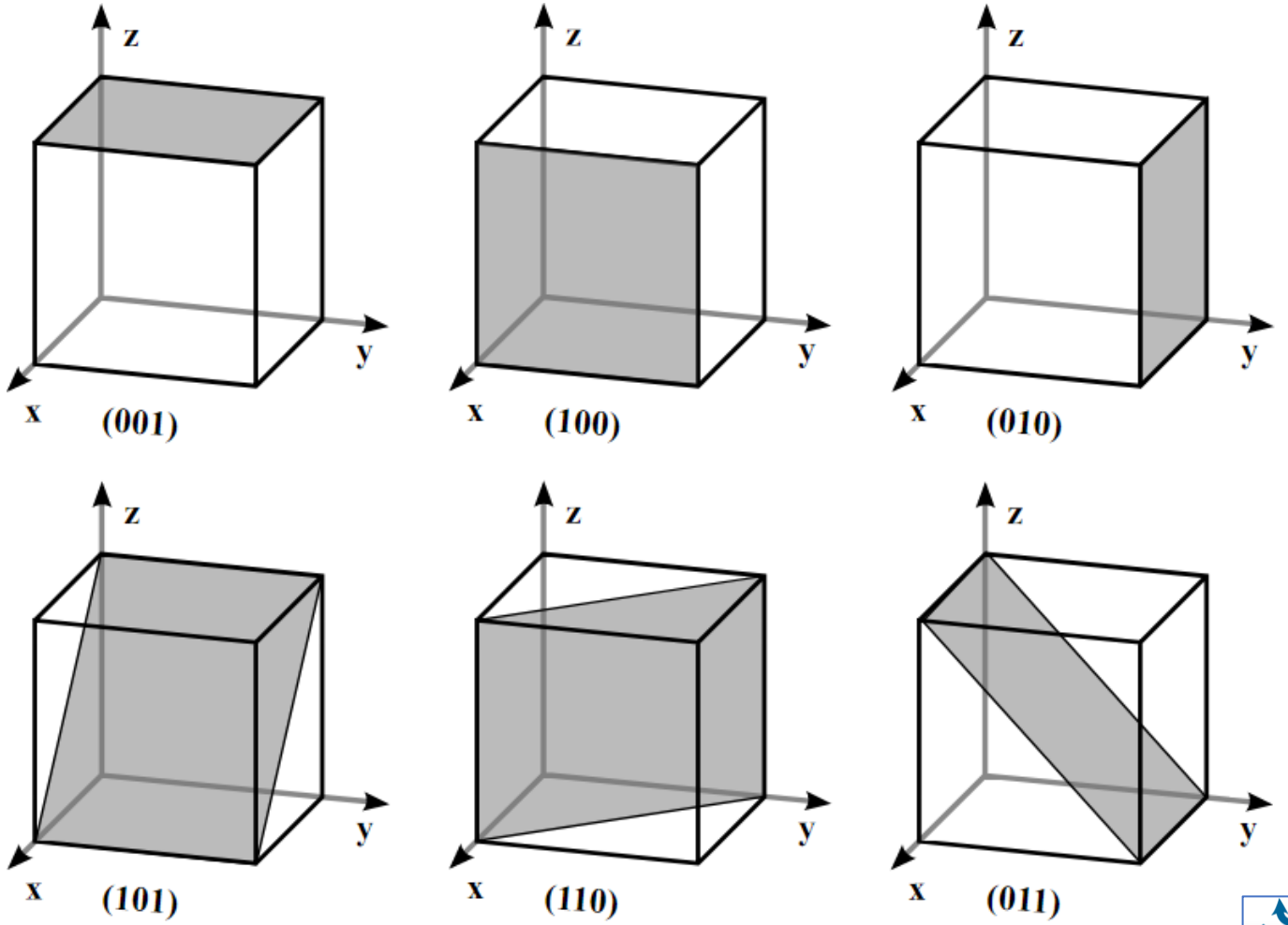
$(1, 1, 1) \rightarrow (111)$



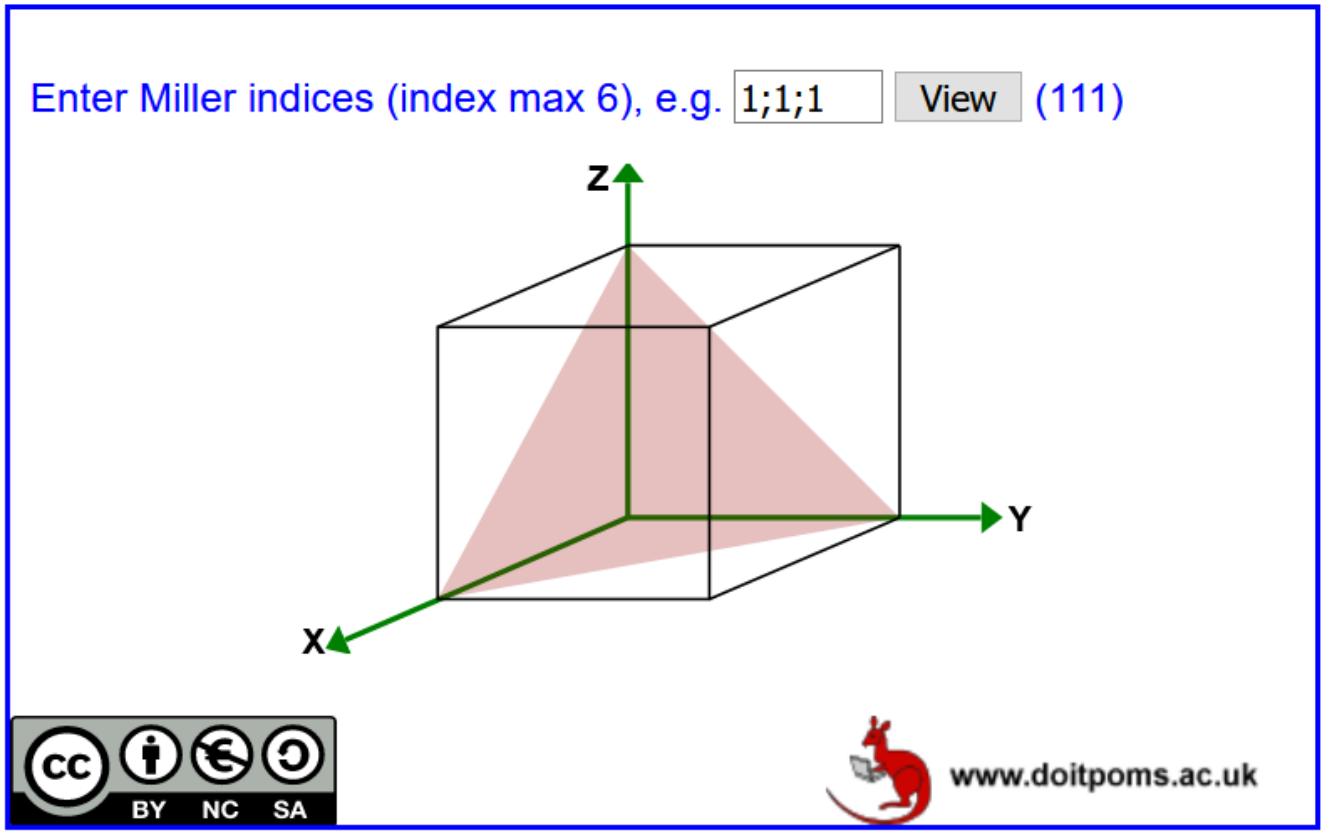
Miller Indices



$$\left(\frac{1}{2}, 1, \infty\right) \rightarrow (210)$$

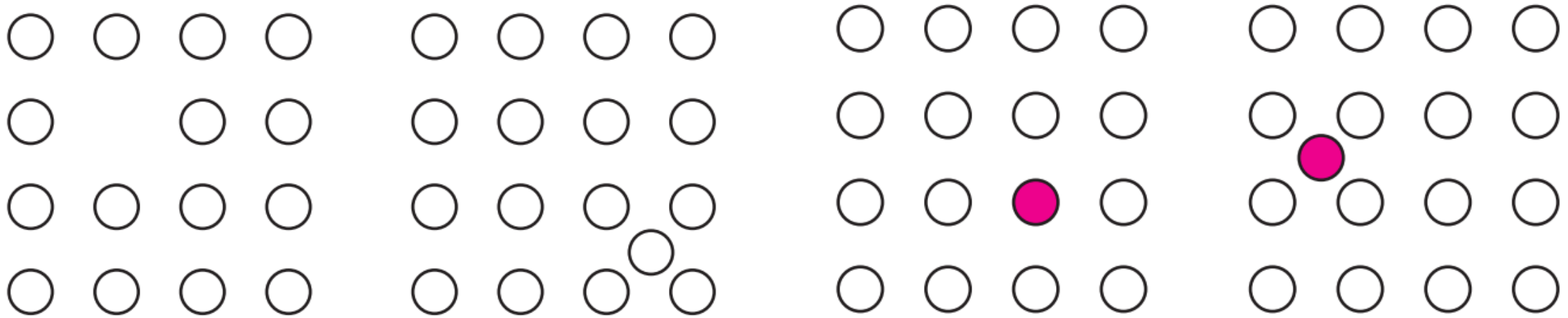


Draw your own lattice planes



https://www.doitpoms.ac.uk/tlplib/miller_indices/lattice_draw.php

Crystal Defects



Point defects in a crystal. (*a*) Vacancy. (*b*) Interstitial. (*c*) Substitutional impurity. (*d*) Interstitial impurity.

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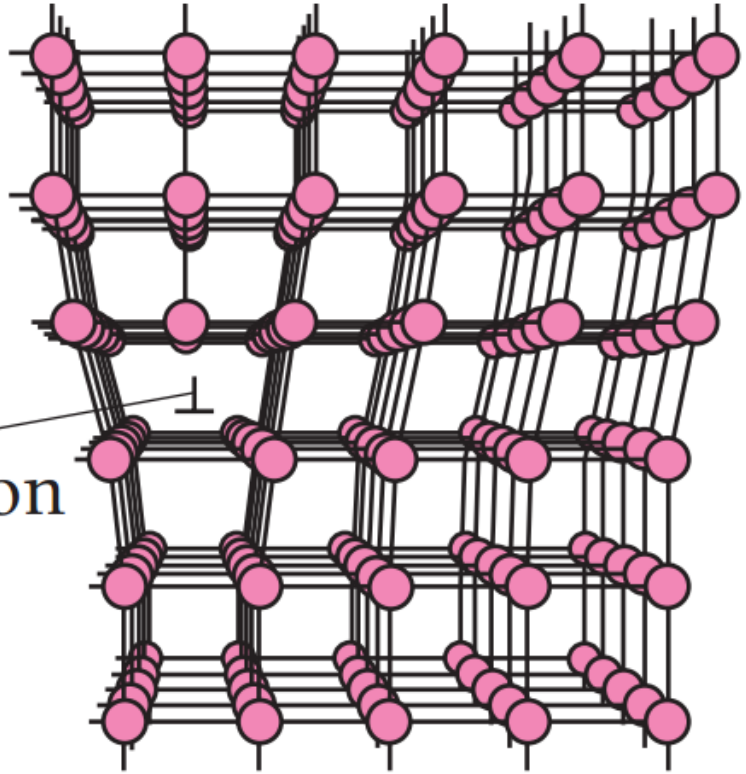
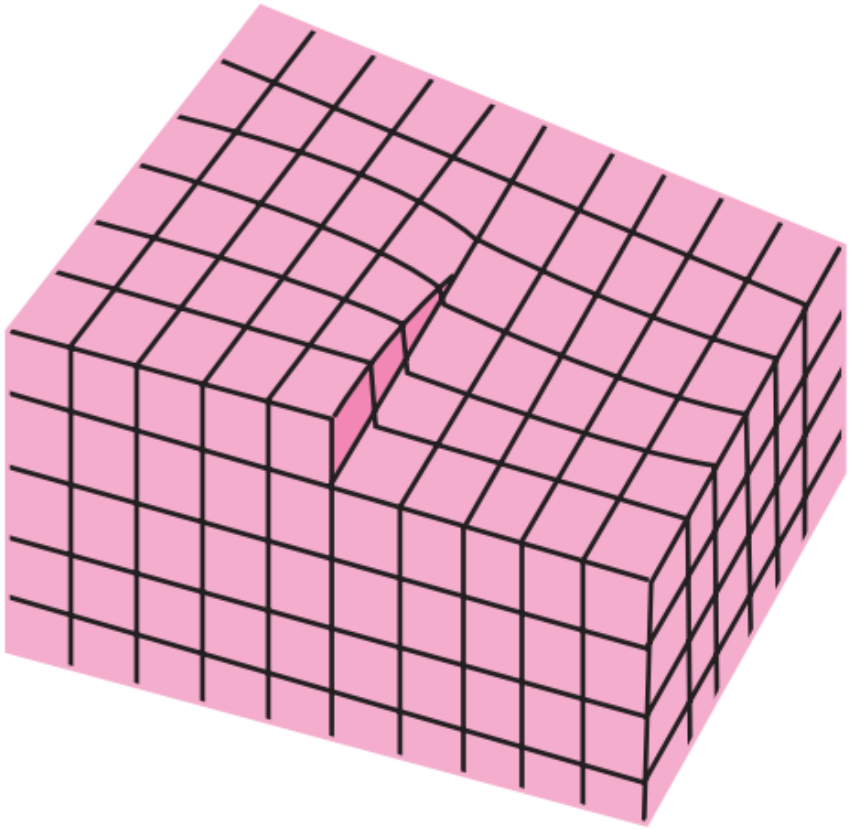
Crystal Defects





A screw dislocation.

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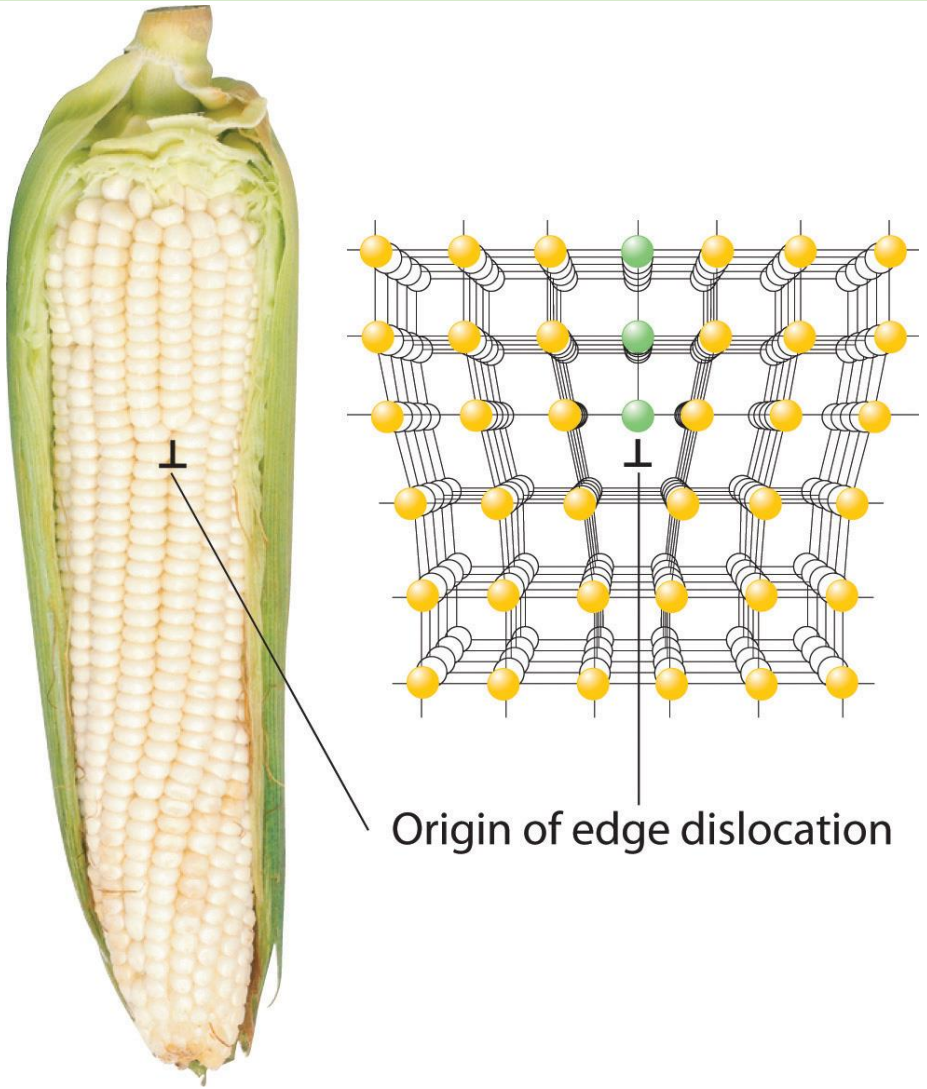
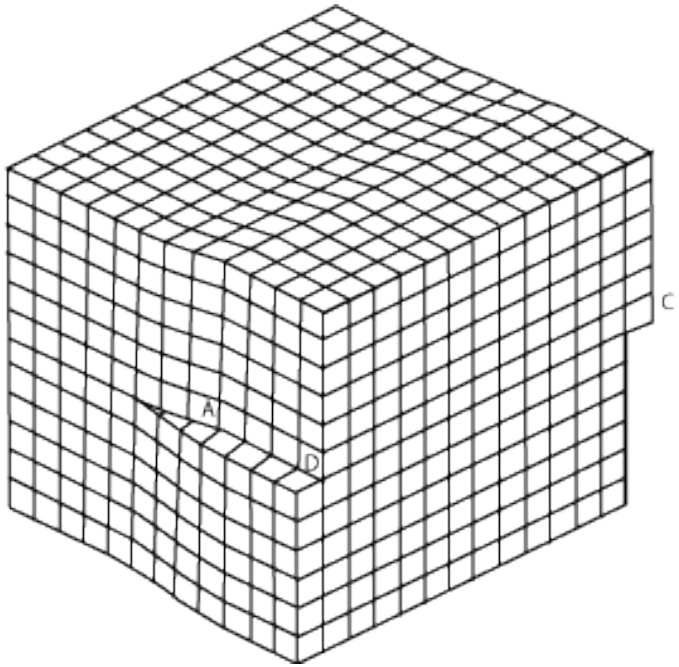
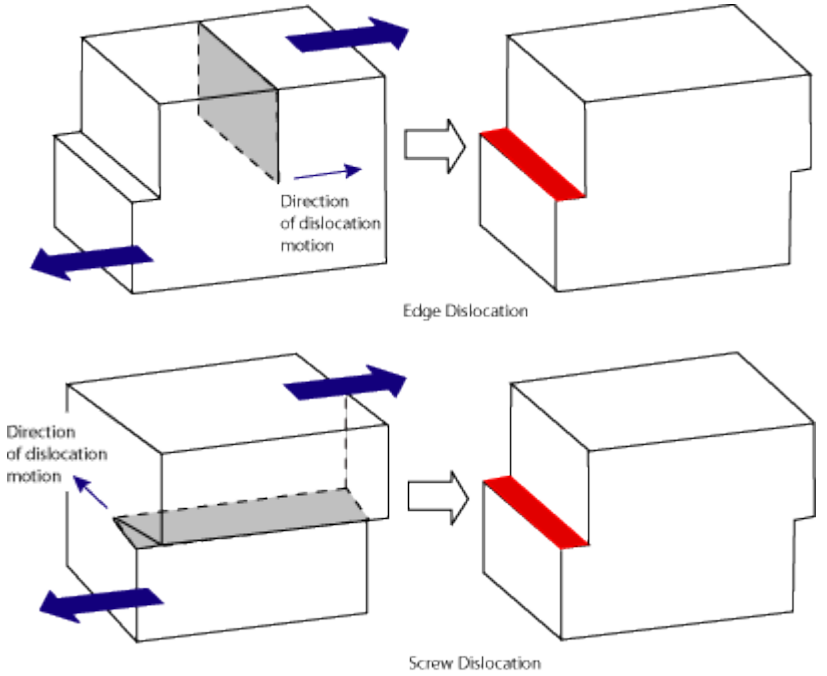
Crystal Defects



Crystal Defects





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