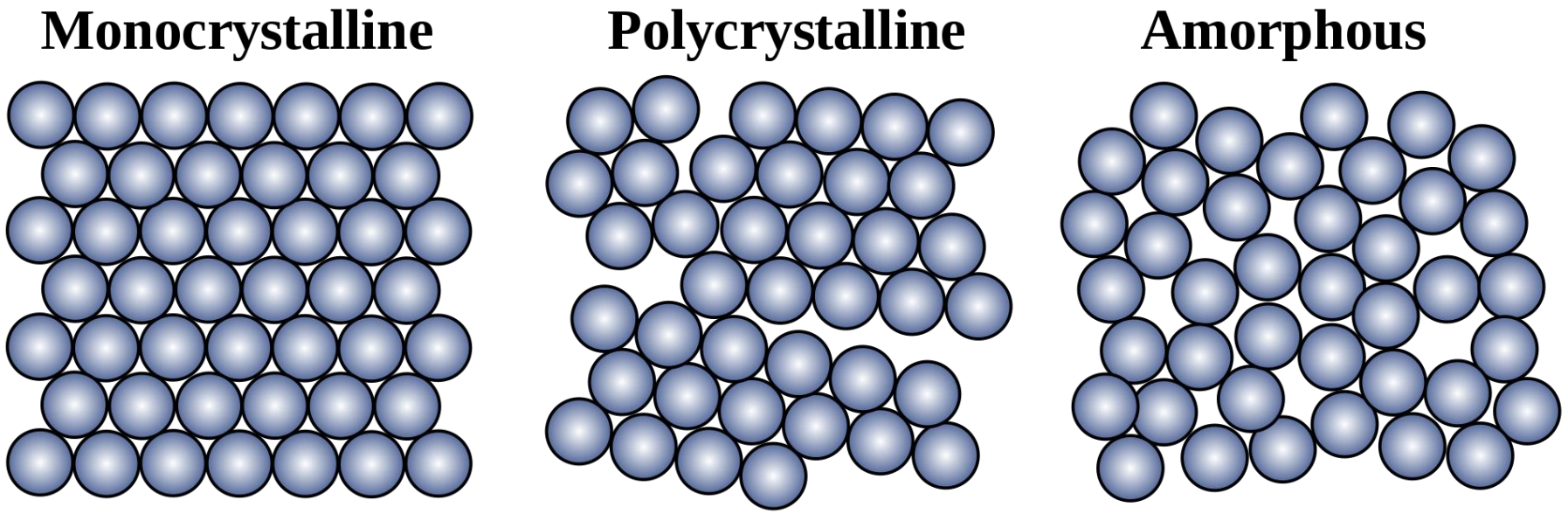
Structure of Matter

Dr Mohammad Abdur Rashid

Classification of solids

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



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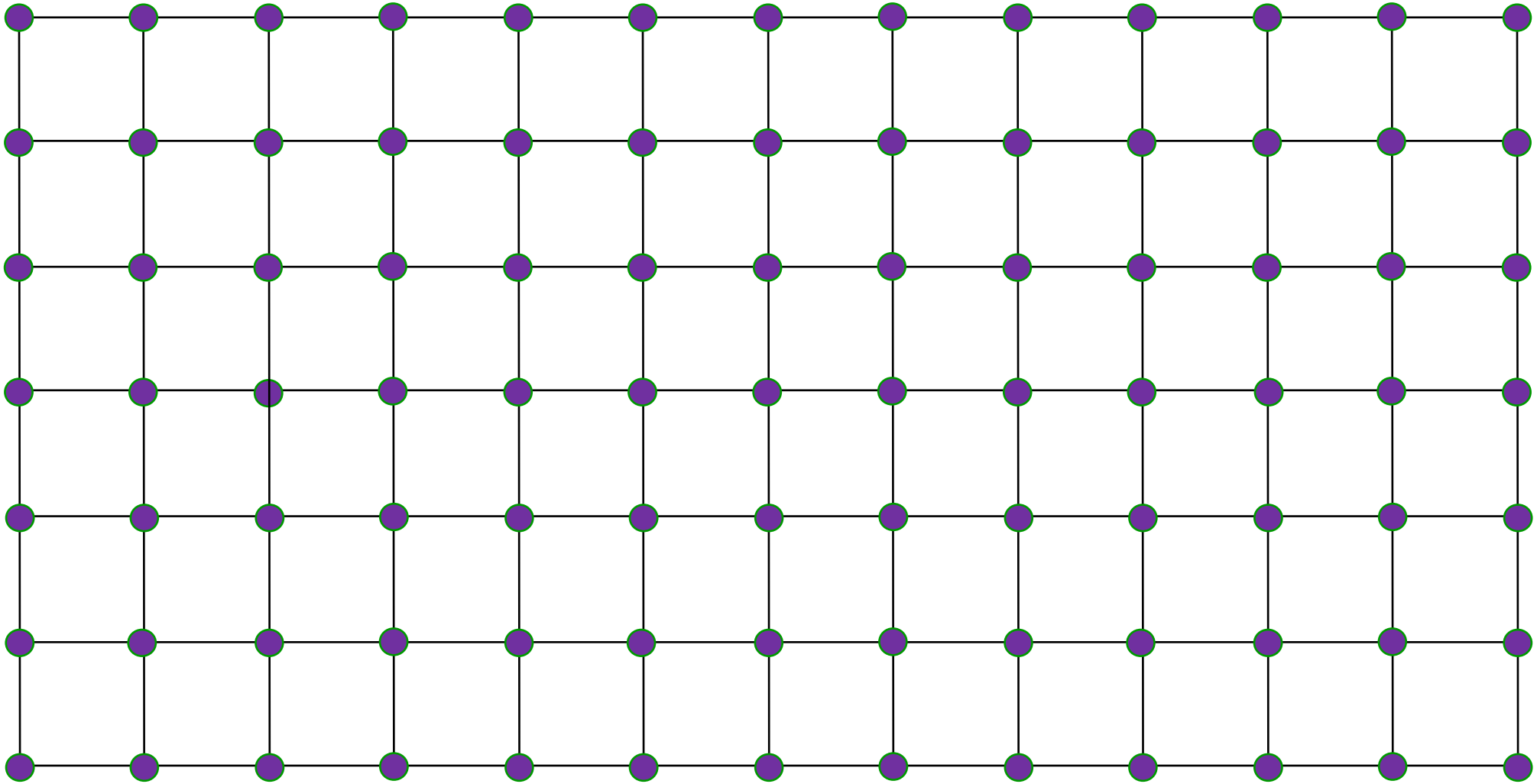
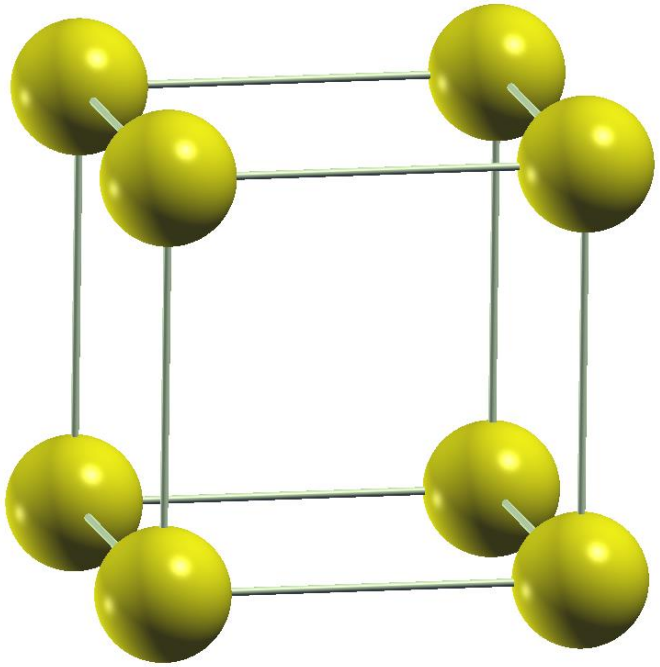
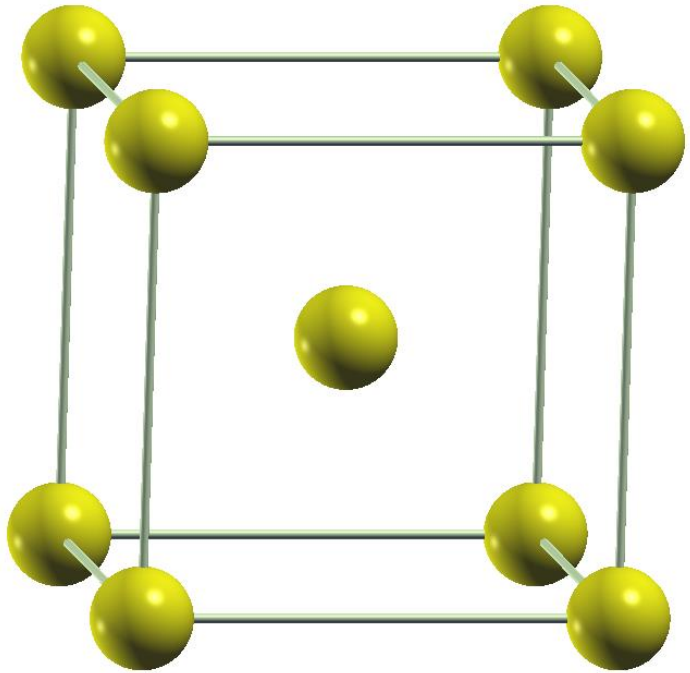
2D Crystal



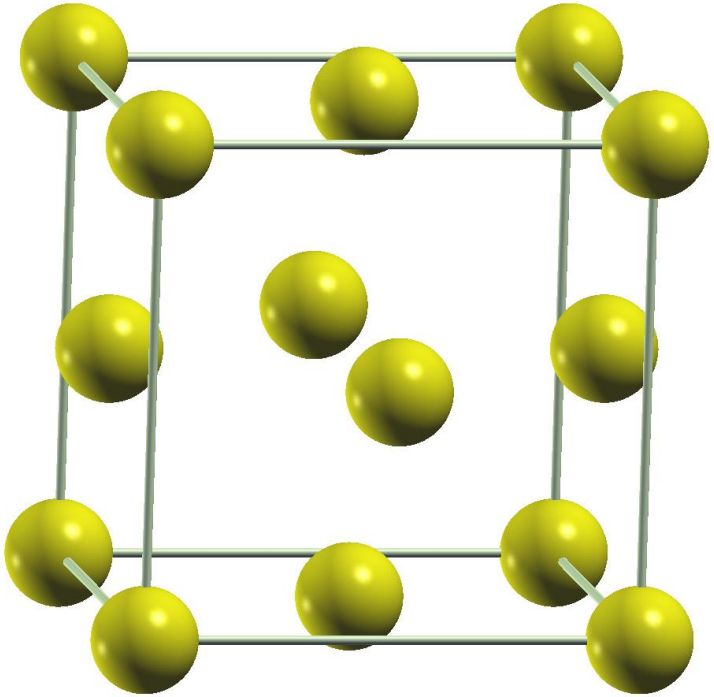
3D Crystal



Simple cubic

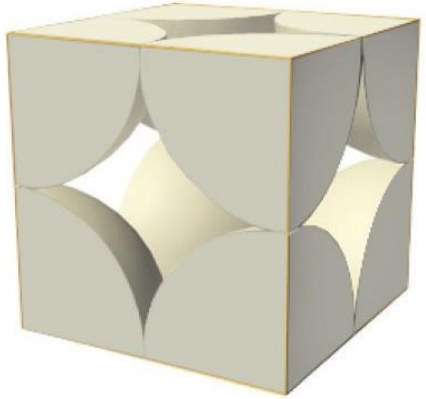


Body-centered cubic

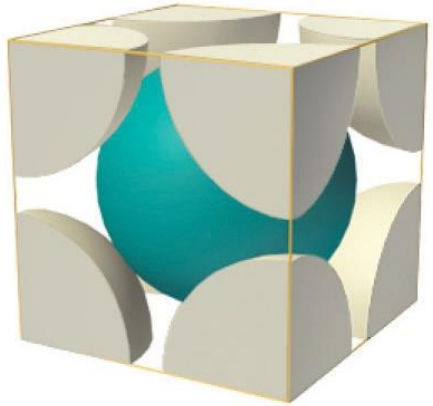


Face-centered cubic

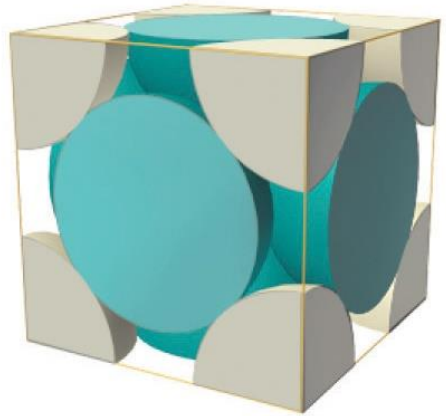
3D Crystal



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.

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:

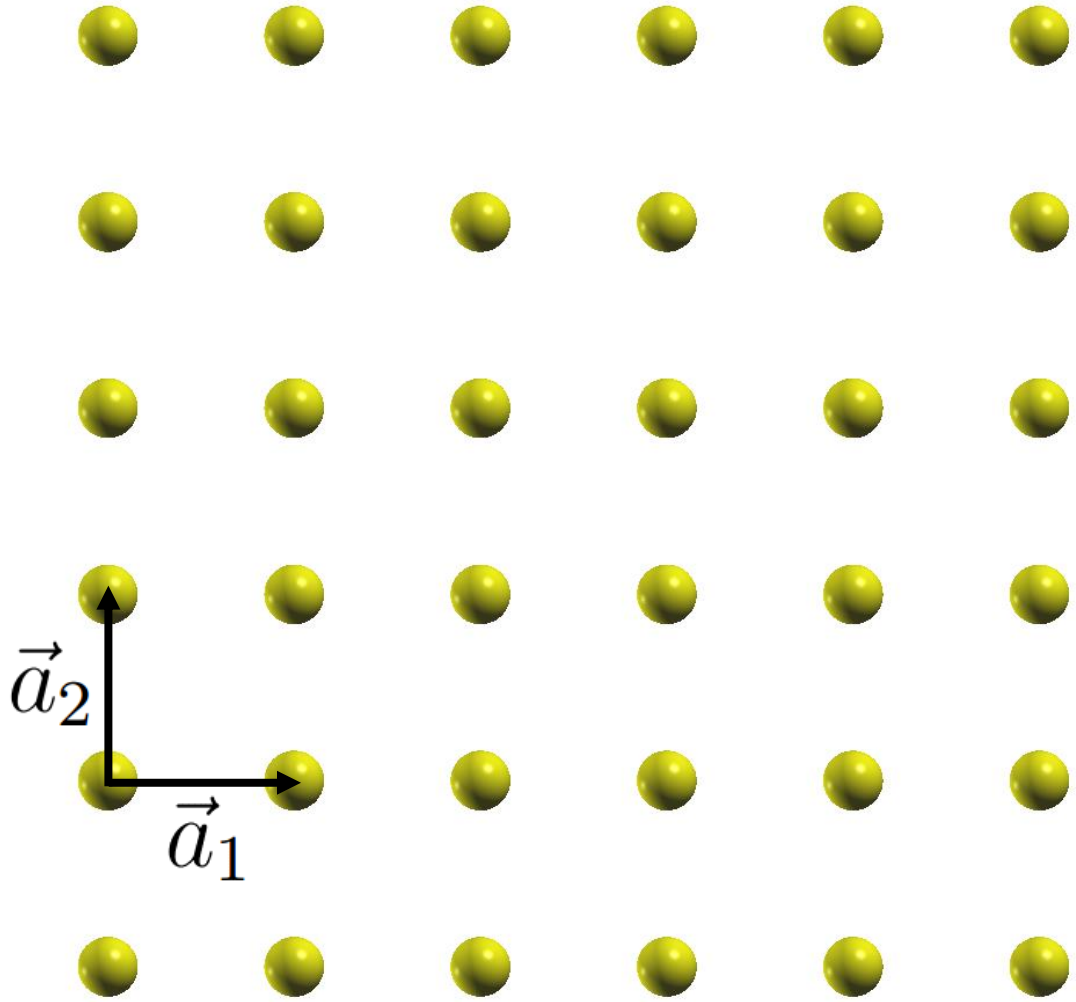
$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$

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

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

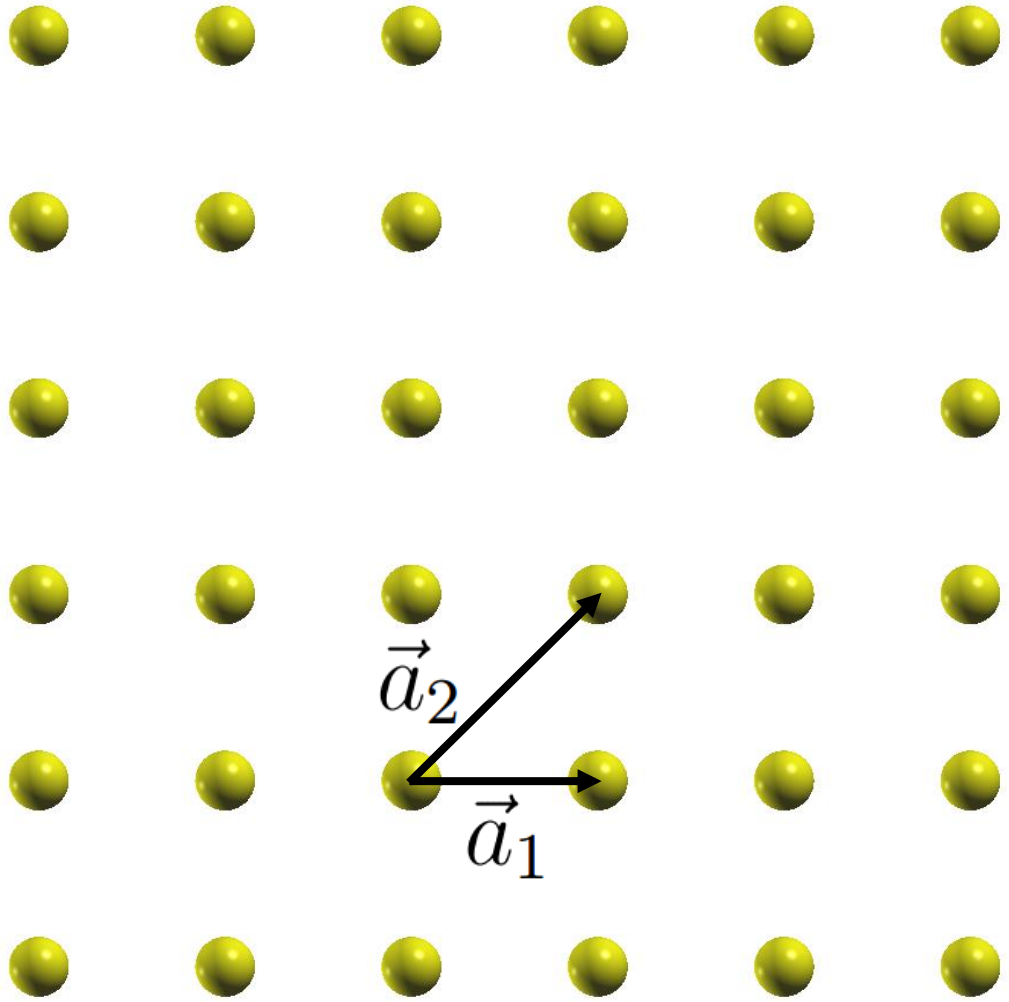
1	0
0	1
1	1
2	2



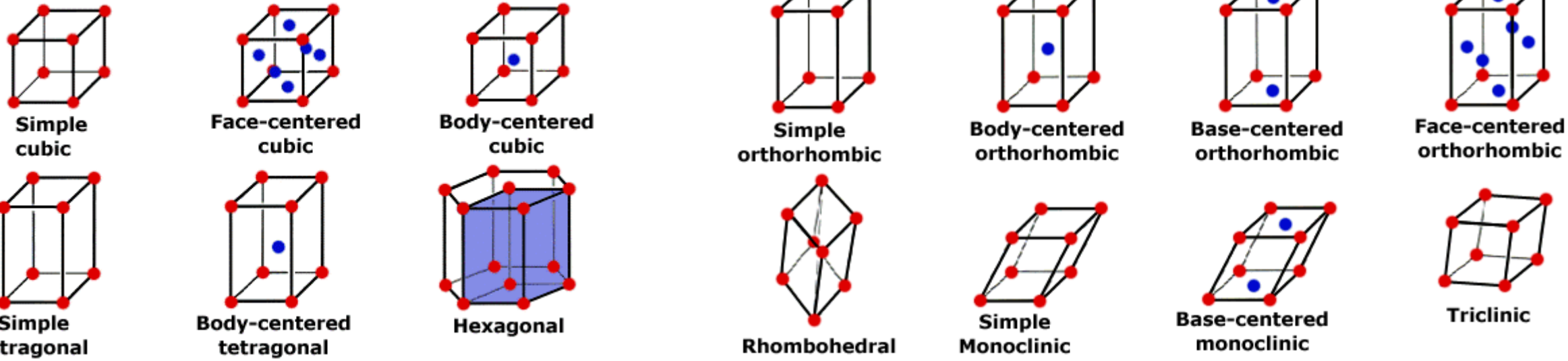
2D Crystal

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

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



Bravais lattice in 3D



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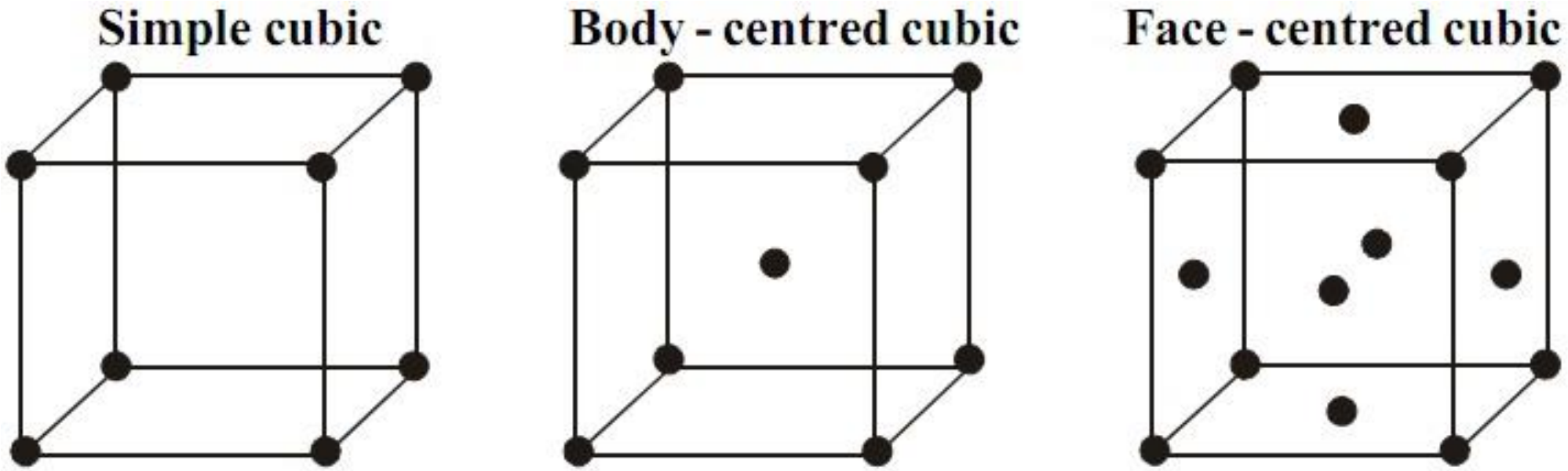
Bravais lattice in 3D



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

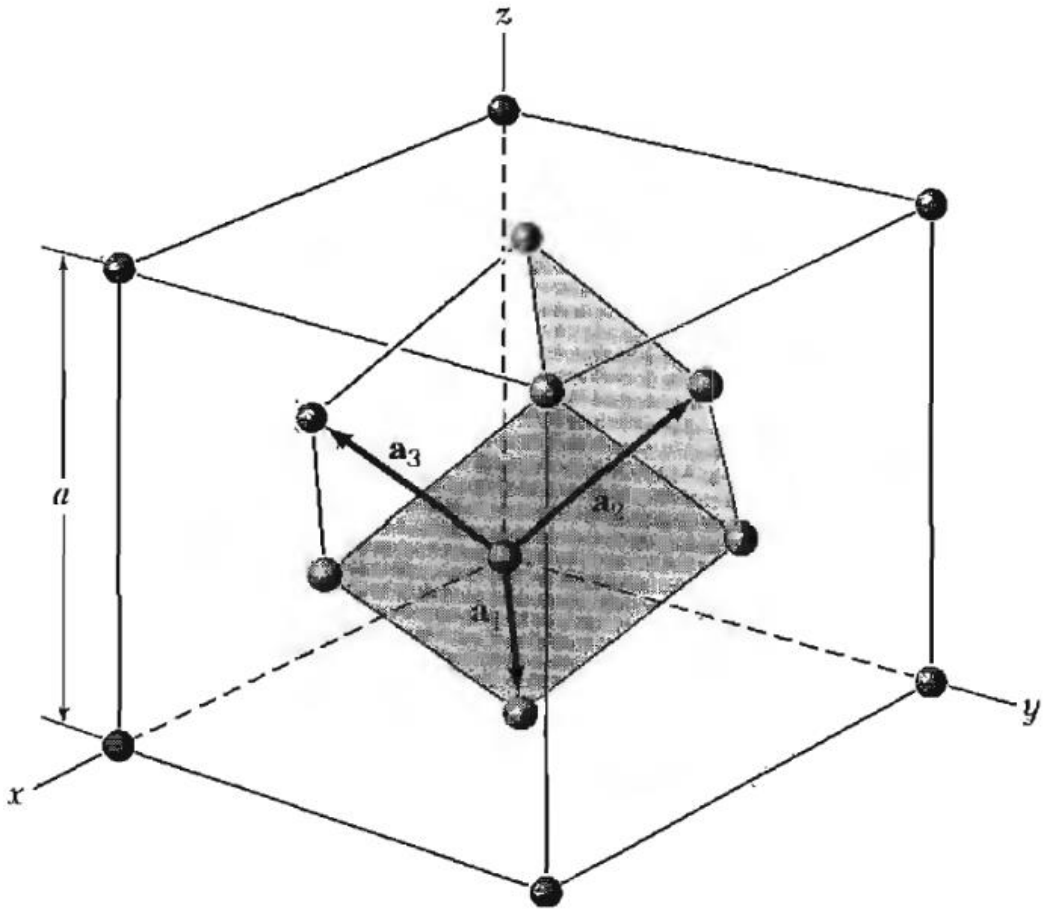
Primitive translational vector of fcc lattice

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

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

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

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



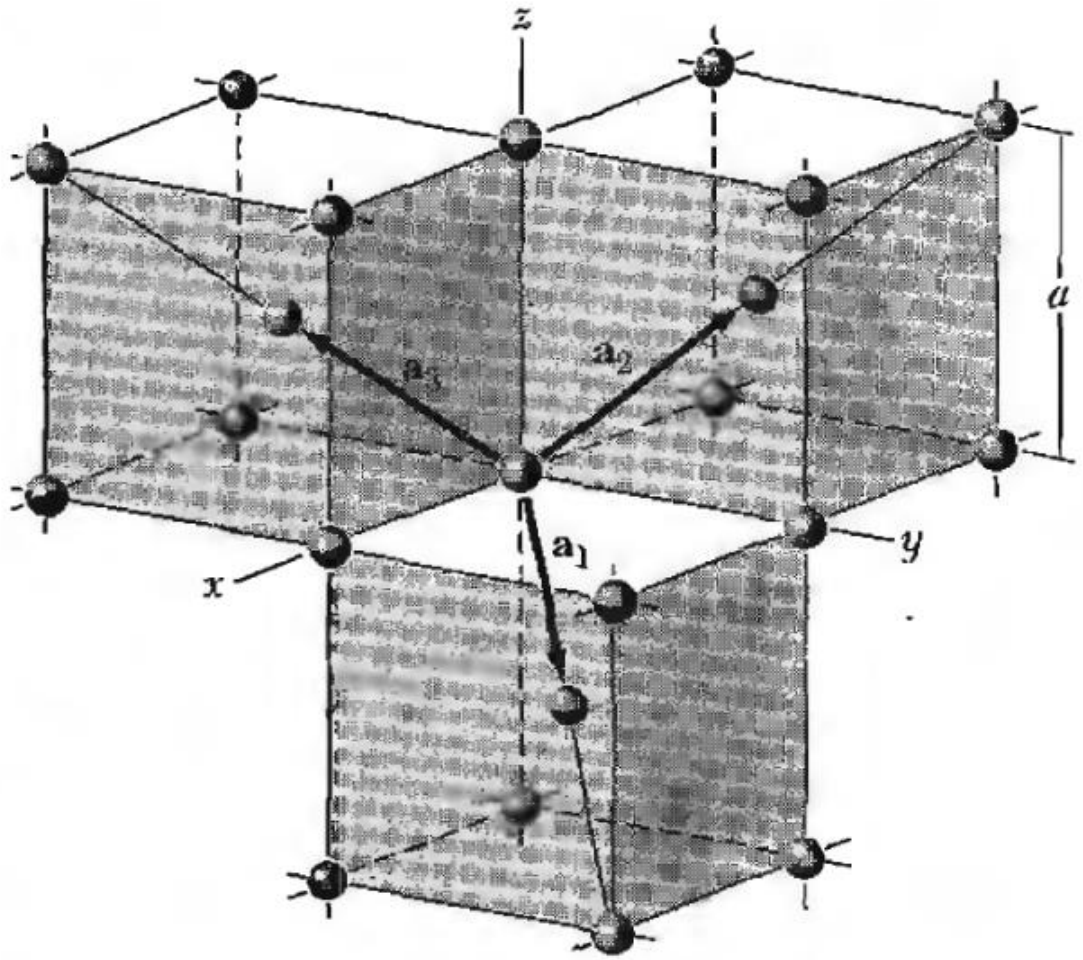
Primitive translational vector of bcc lattice

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

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

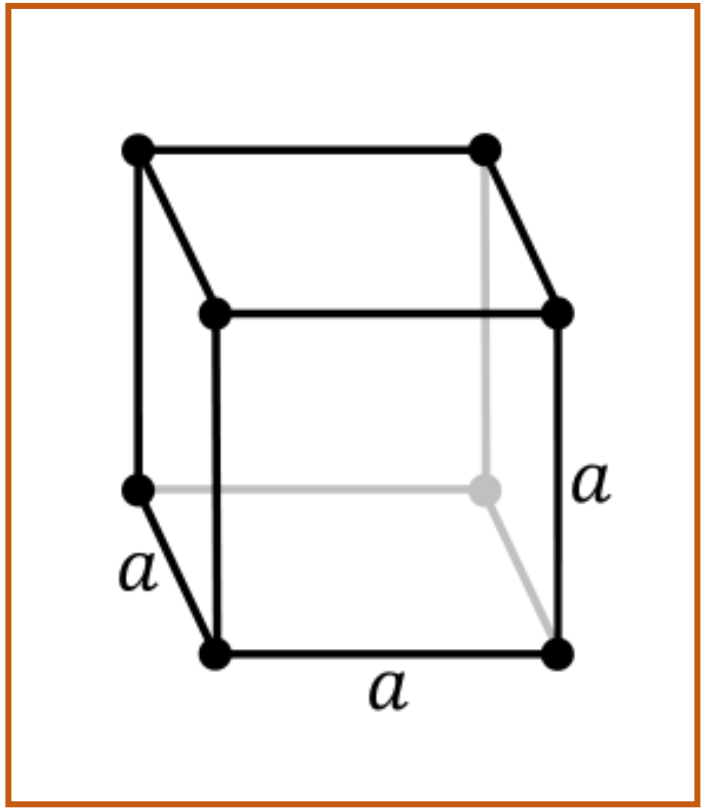
$$\vec{a}_3 = \frac{a}{2}(\hat{z} + \hat{x} - \hat{y})$$

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



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.



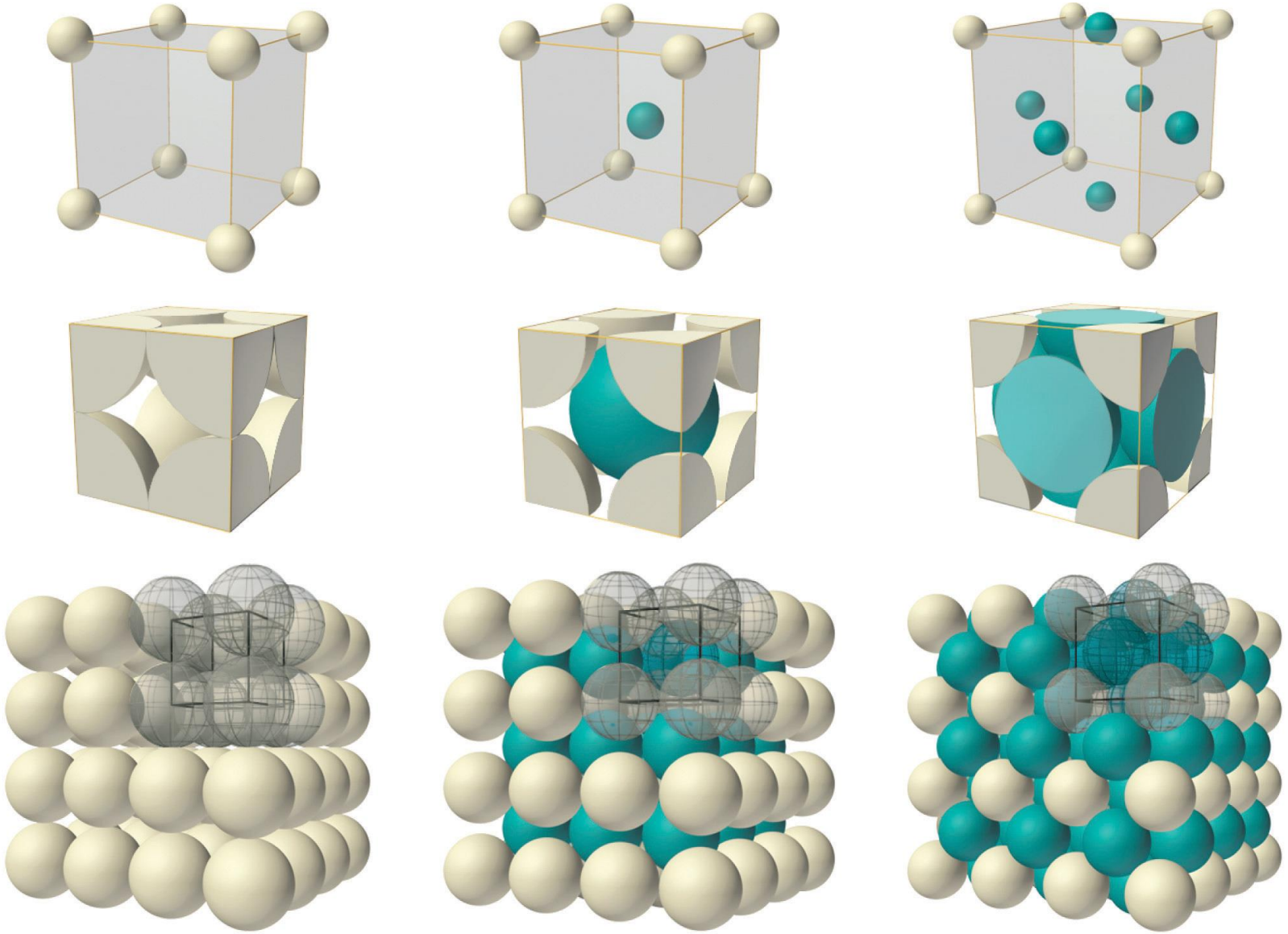
Primitive lattice cell

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

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

3D view showing the number of atoms per unit cell

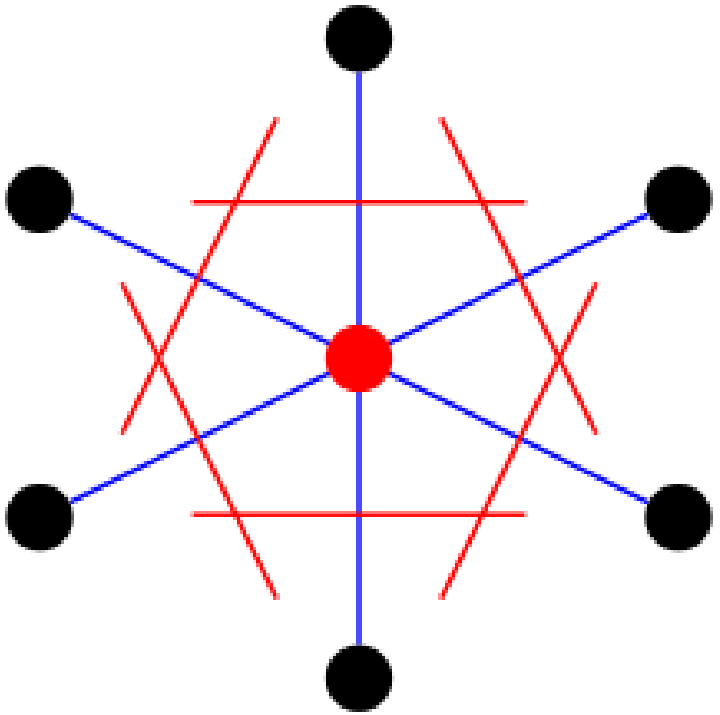


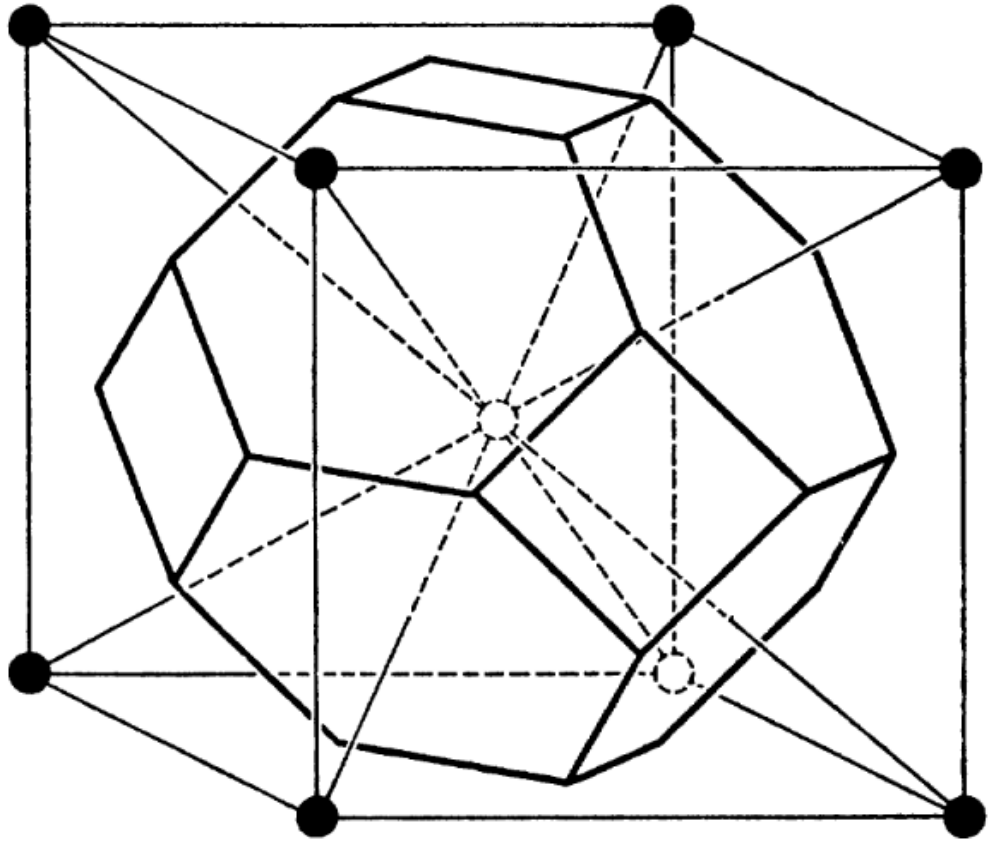
(a) Simple cubic (b) Body-centered cubic (c) Face-centered cubic

Characteristics of cubic lattices

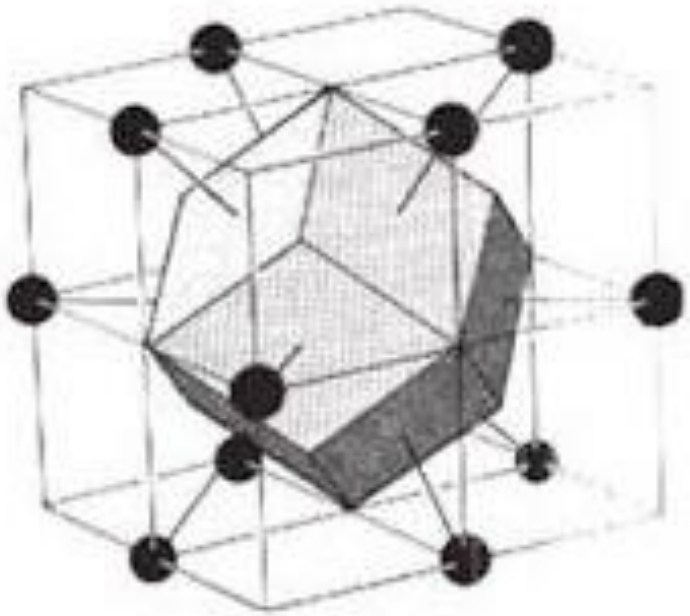
	Simple	Body-centered	Face-centered
Volume, conventional cell	a^3	a^3	a^3
Lattice points per cell	1	2	4
Volume, primitive cell	a^3	$\frac{1}{2}a^3$	$\frac{1}{4}a^3$
Lattice points per unit volume	$1/a^3$	$2/a^3$	$4/a^3$
Number of nearest neighbors	6	8	12
Nearest-neighbor distance	a	$3^{1/2}\,a/2 = 0.866a$	$a/2^{1/2} = 0.707a$
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

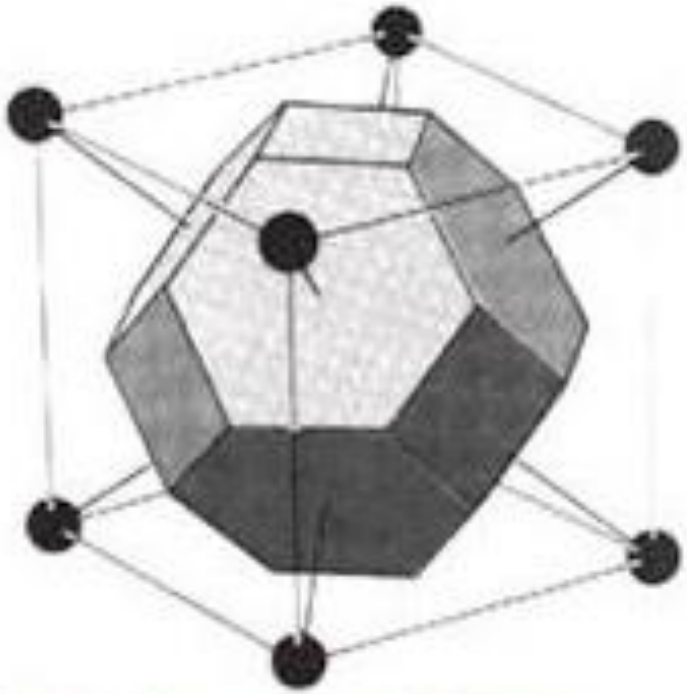




Wigner-Seitz cell



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.

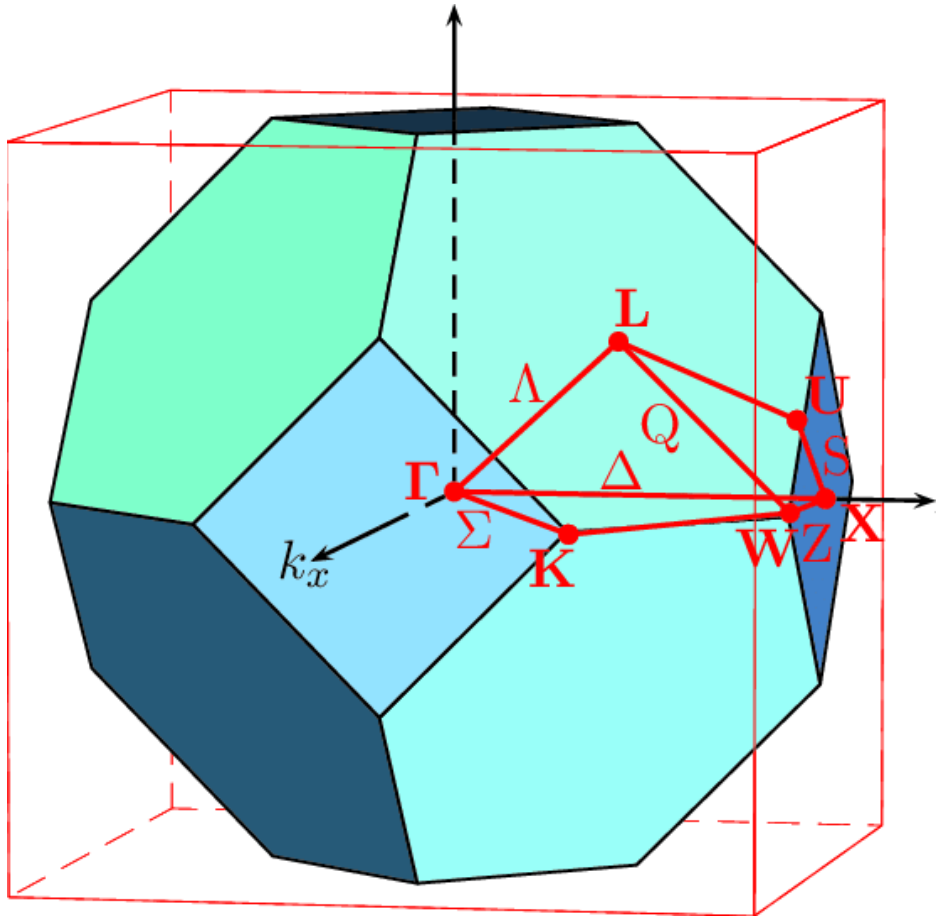
The reciprocal lattice to an fcc lattice is the bcc lattice and vice versa.

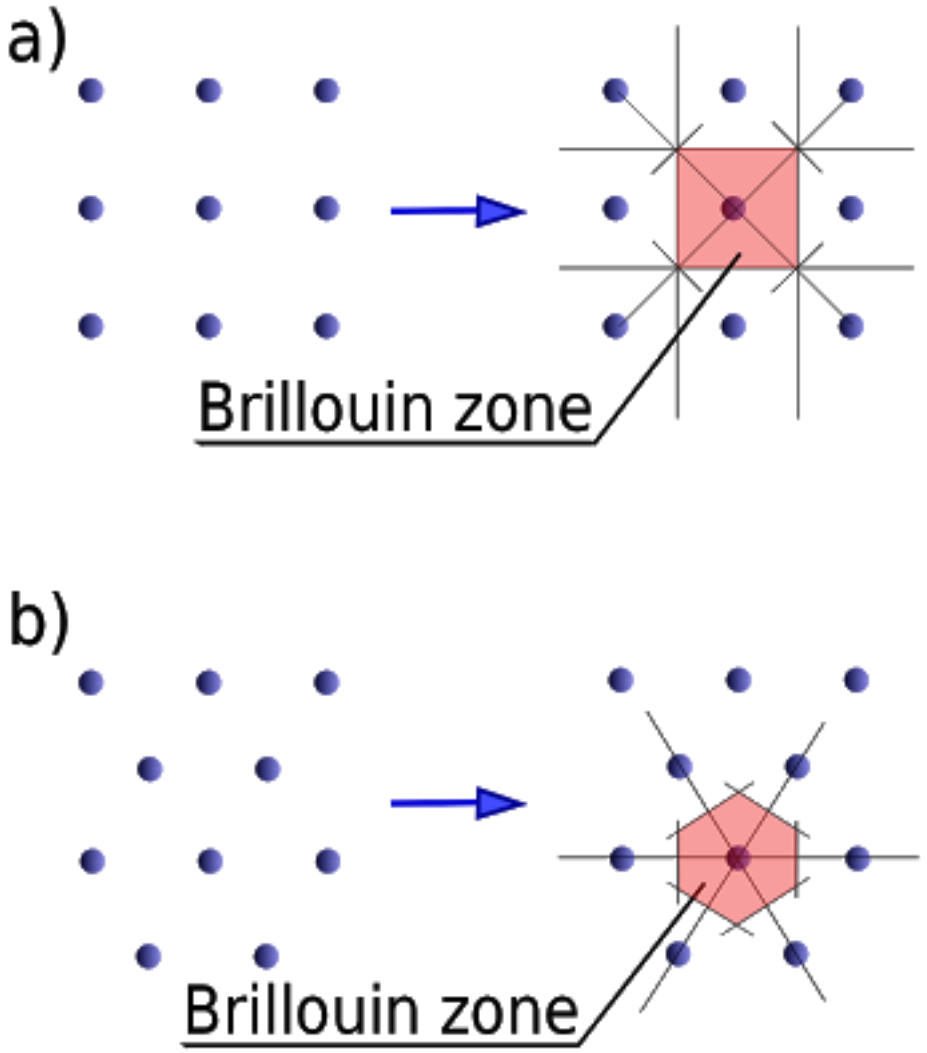
$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

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

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

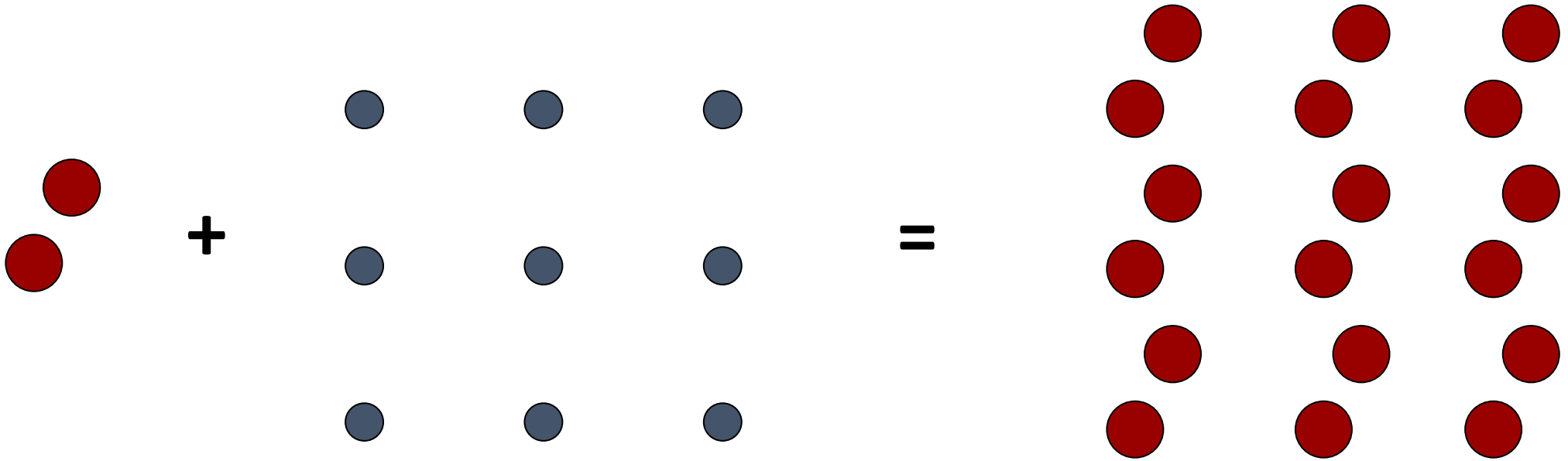
Brillouin zone



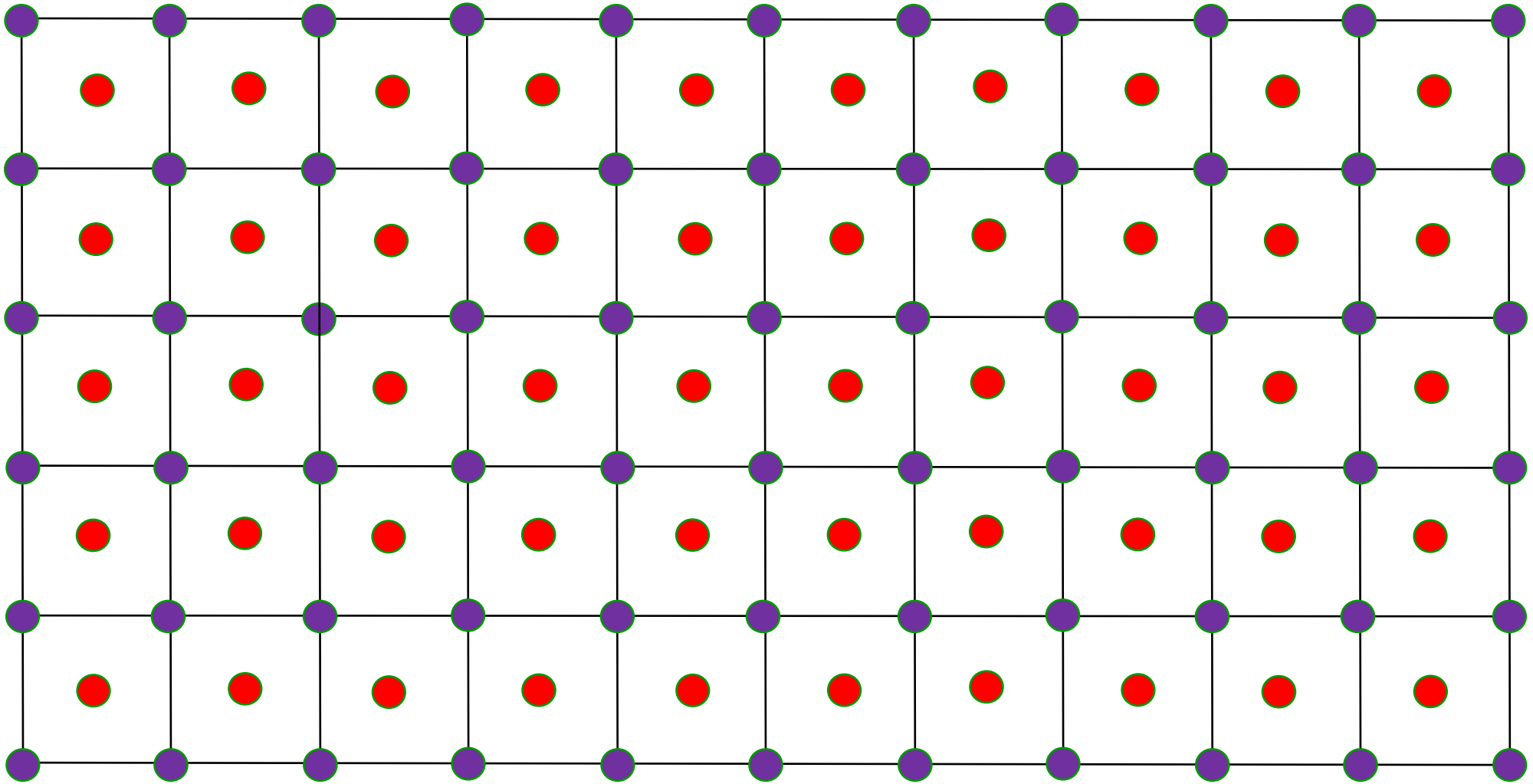


Crystal structure

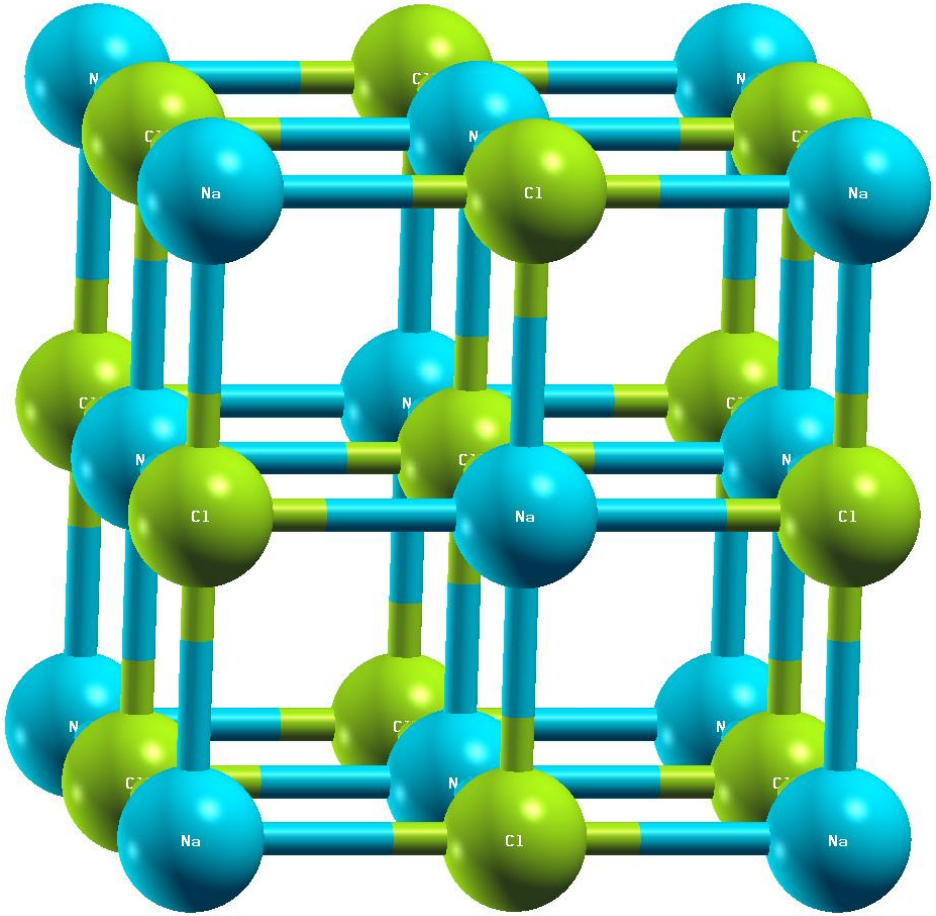
basis + lattice = crystal structure

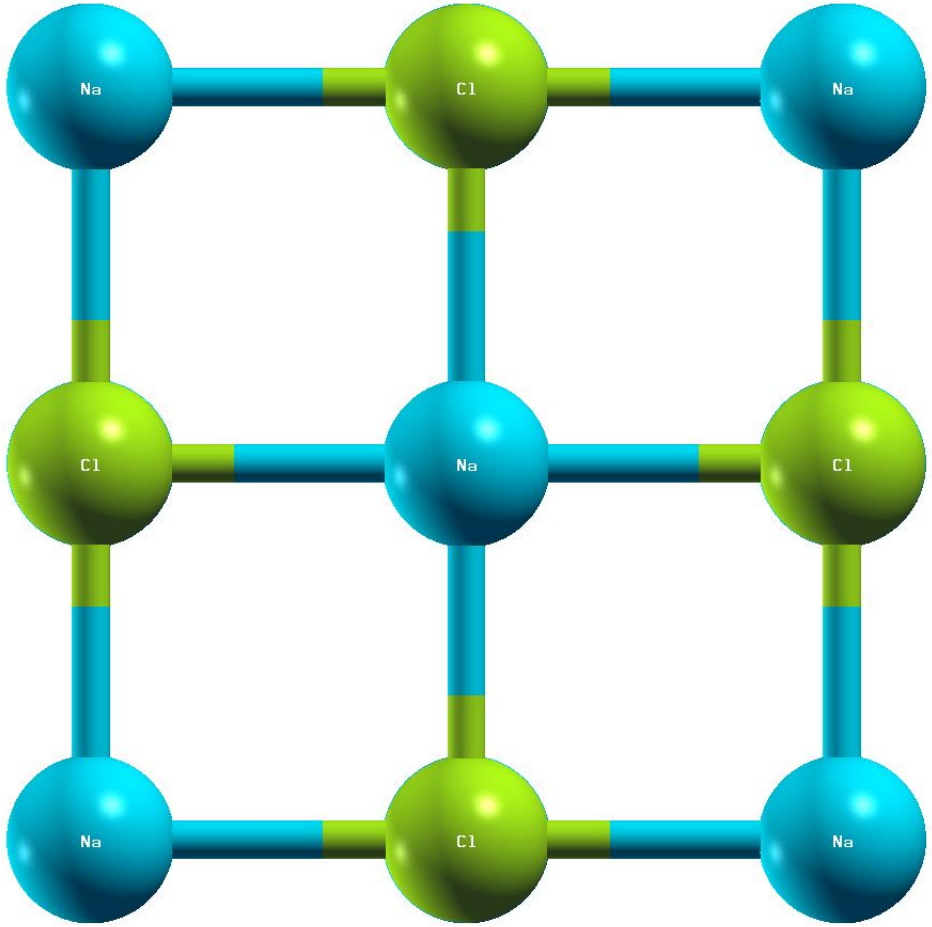


Crystal structure

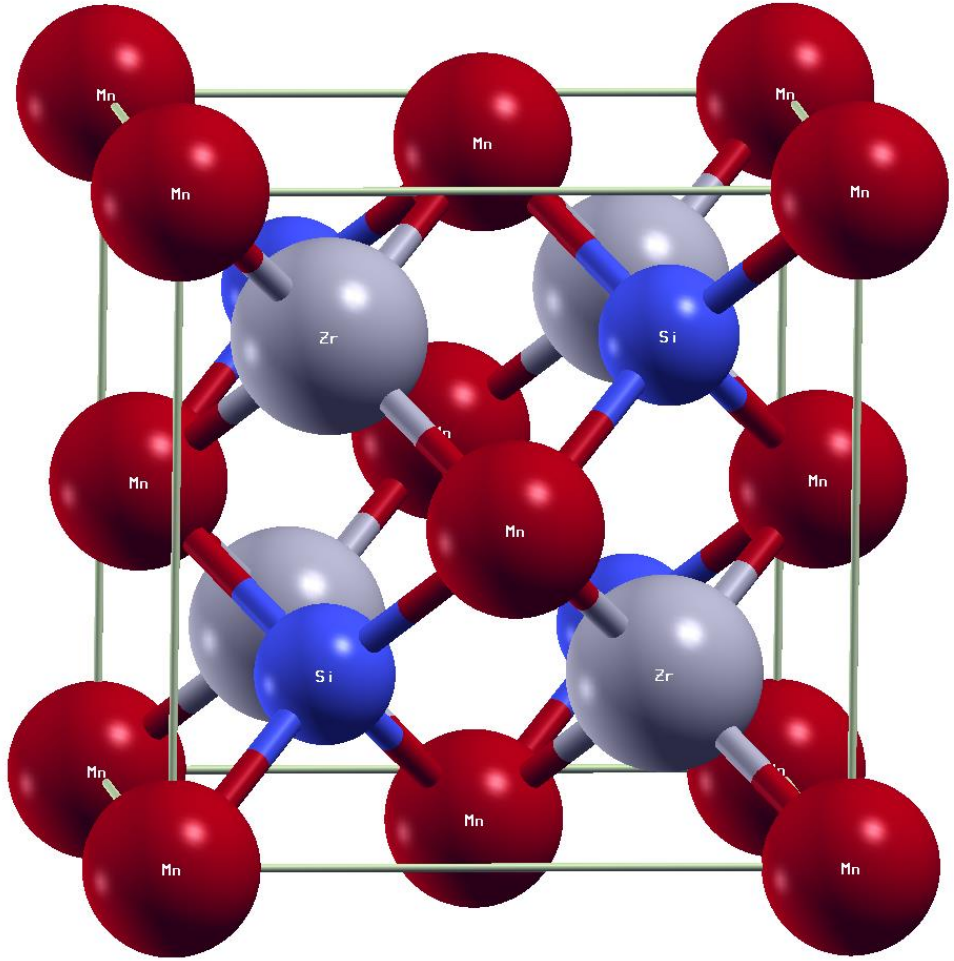


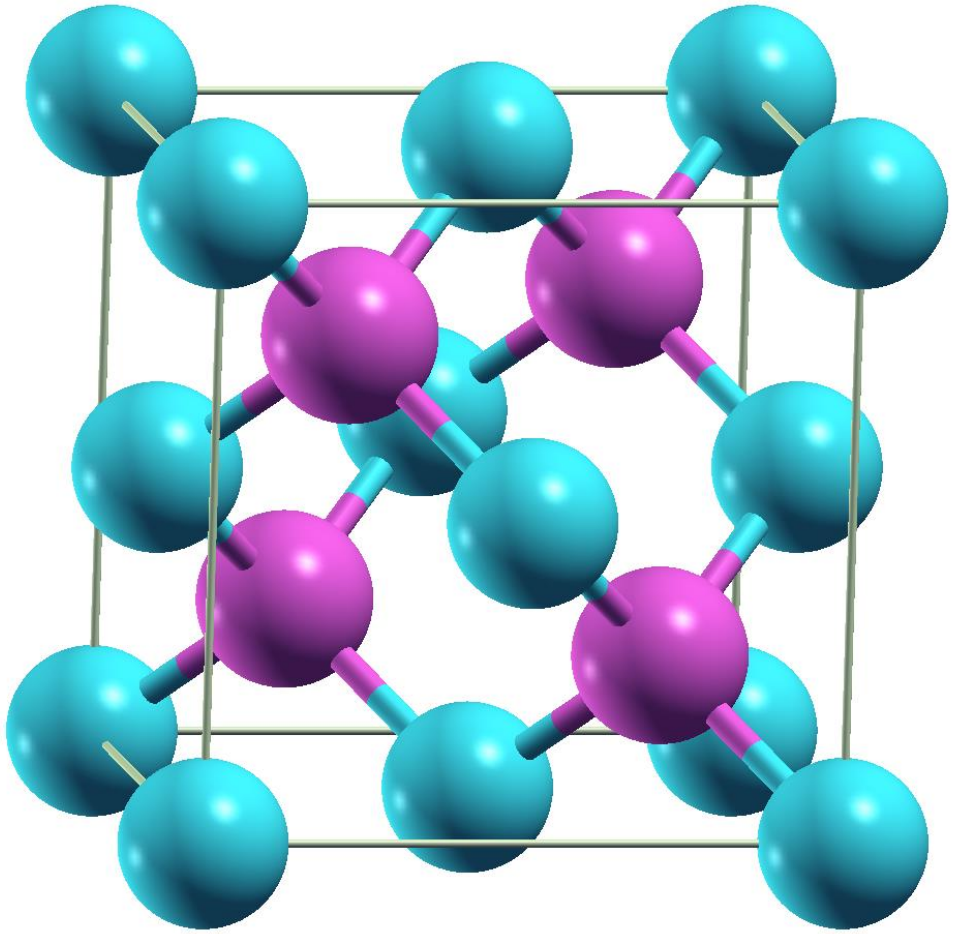
Crystal structure



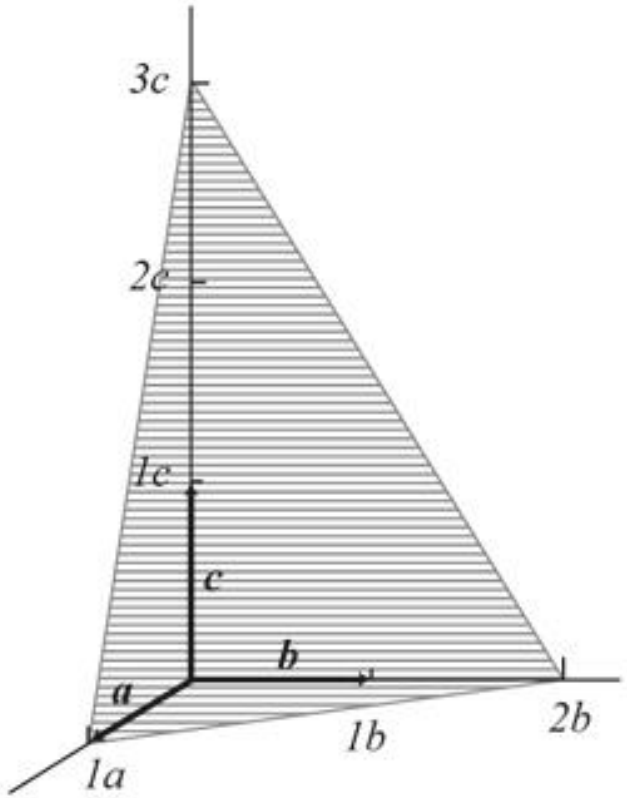


Crystal structure





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

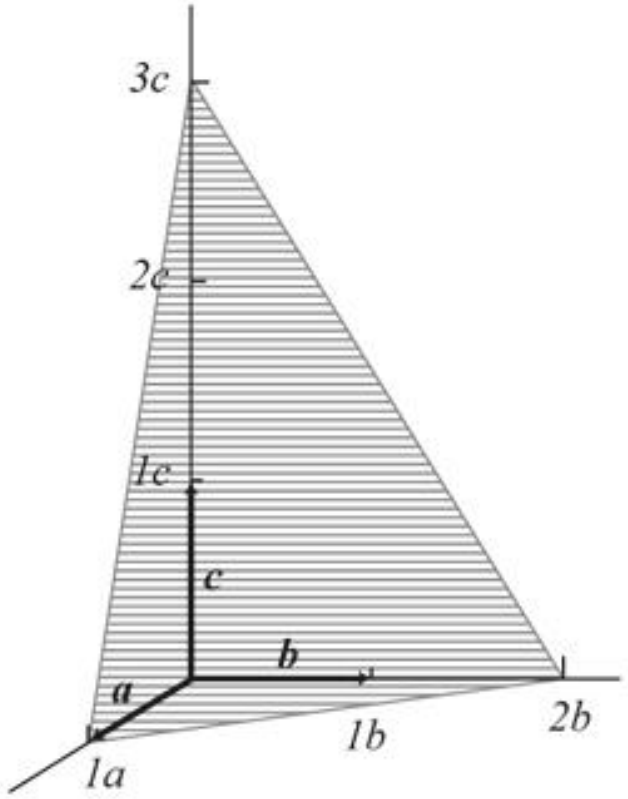
$$h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$$

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

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



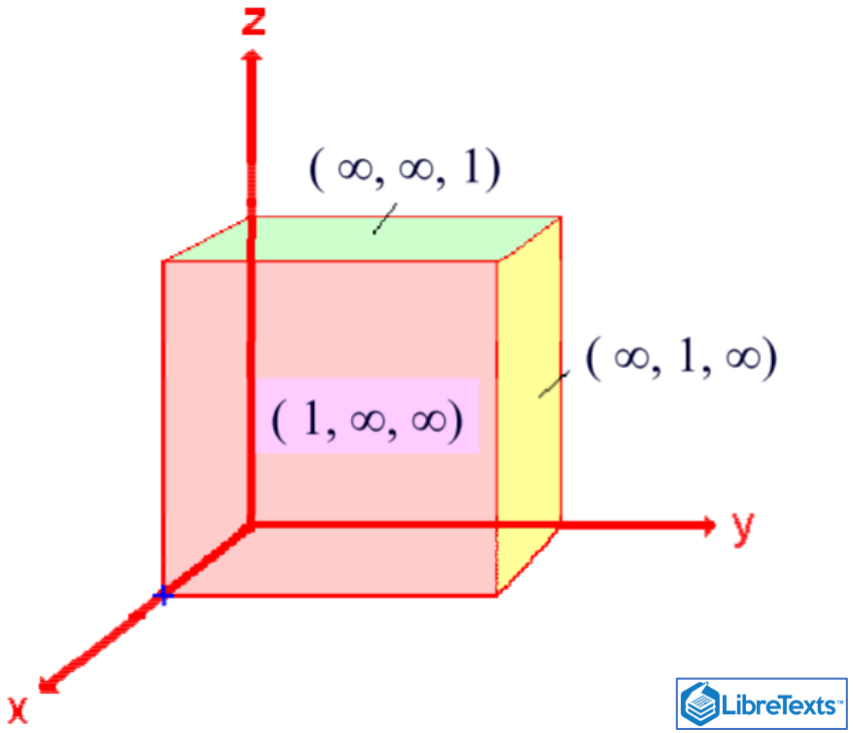
Miller Indices

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

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

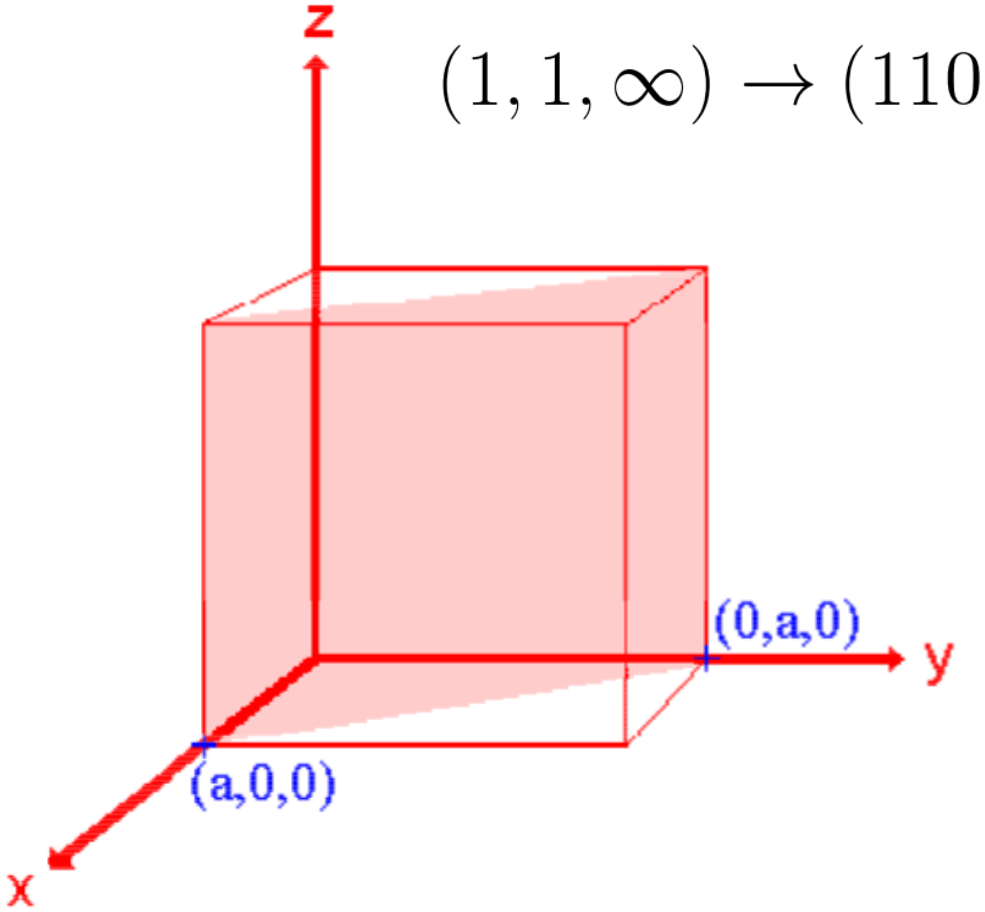
For Green Face: $\left(\frac{1}{\infty}, \frac{1}{\infty}, \frac{1}{1}\right) \rightarrow (001)$

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

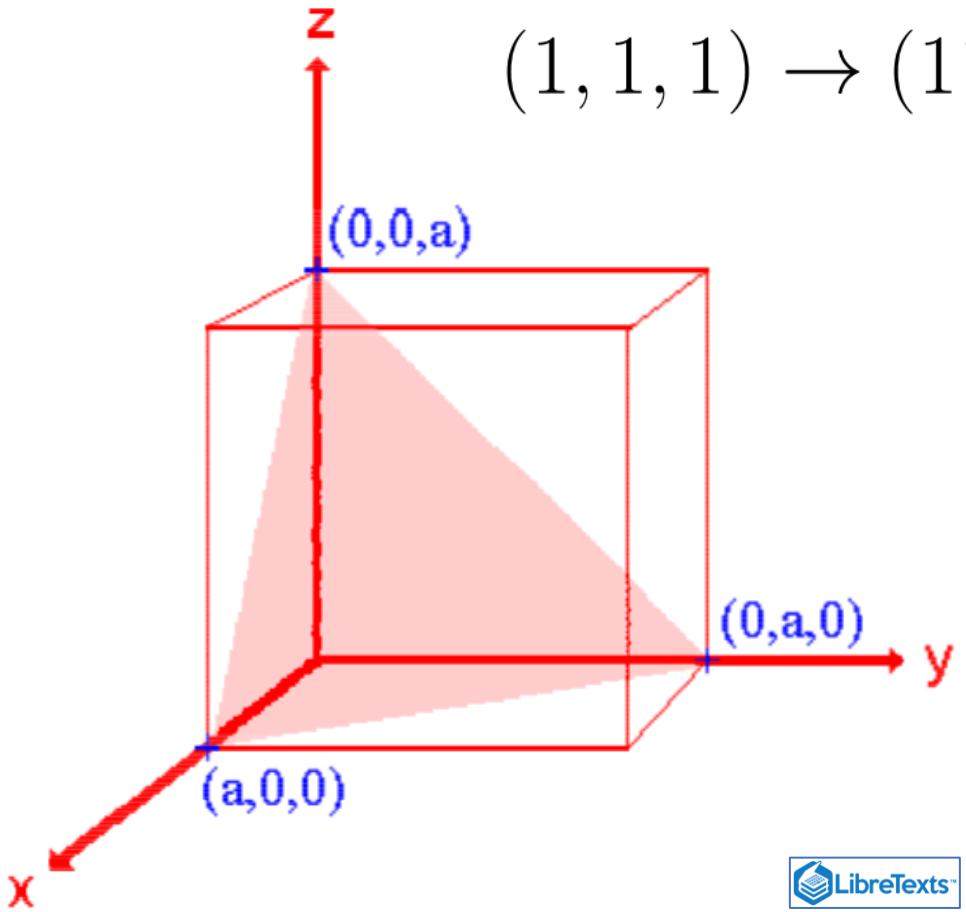


Miller Indices

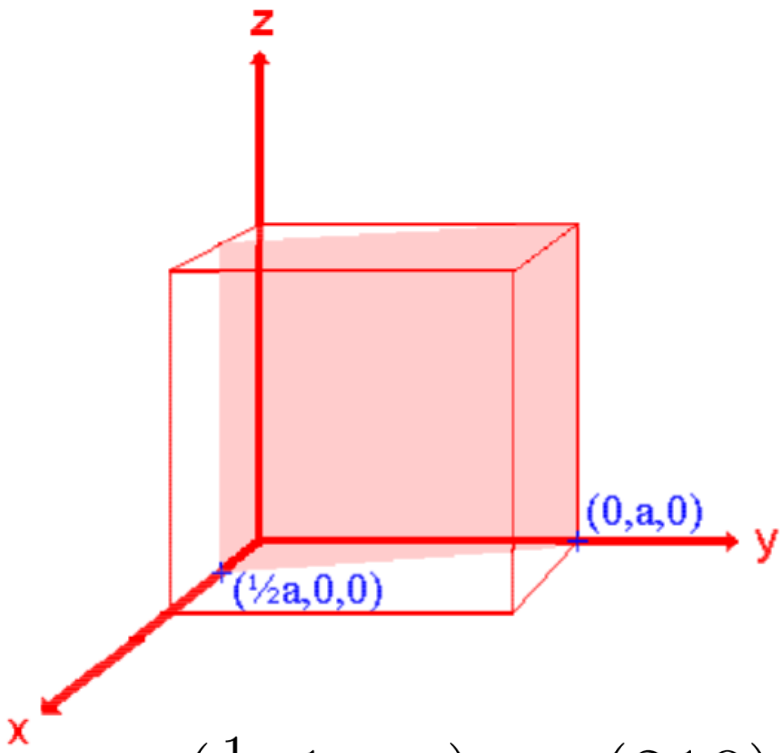
$(1, 1, \infty) \rightarrow (110)$



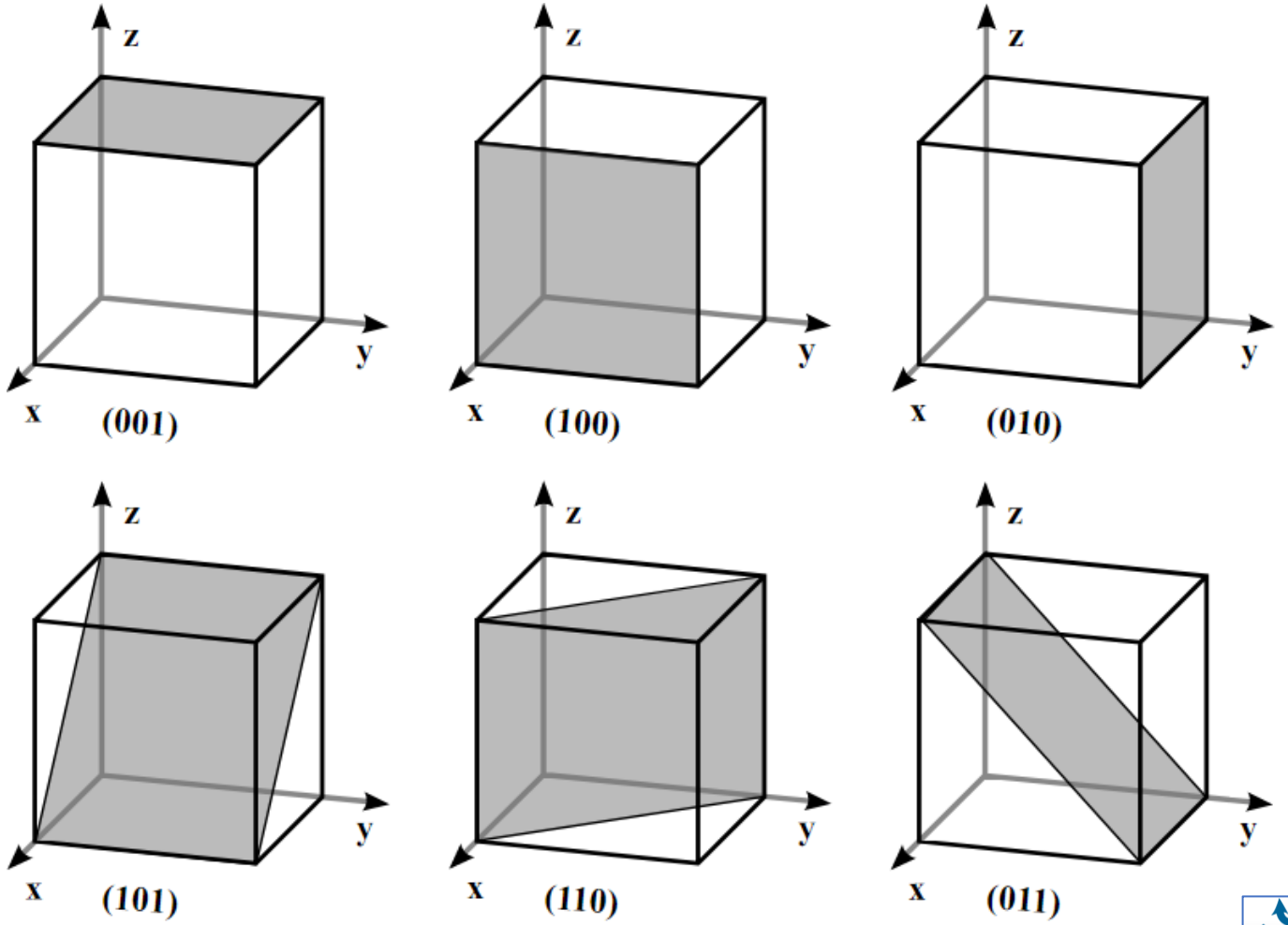
$(1, 1, 1) \rightarrow (111)$



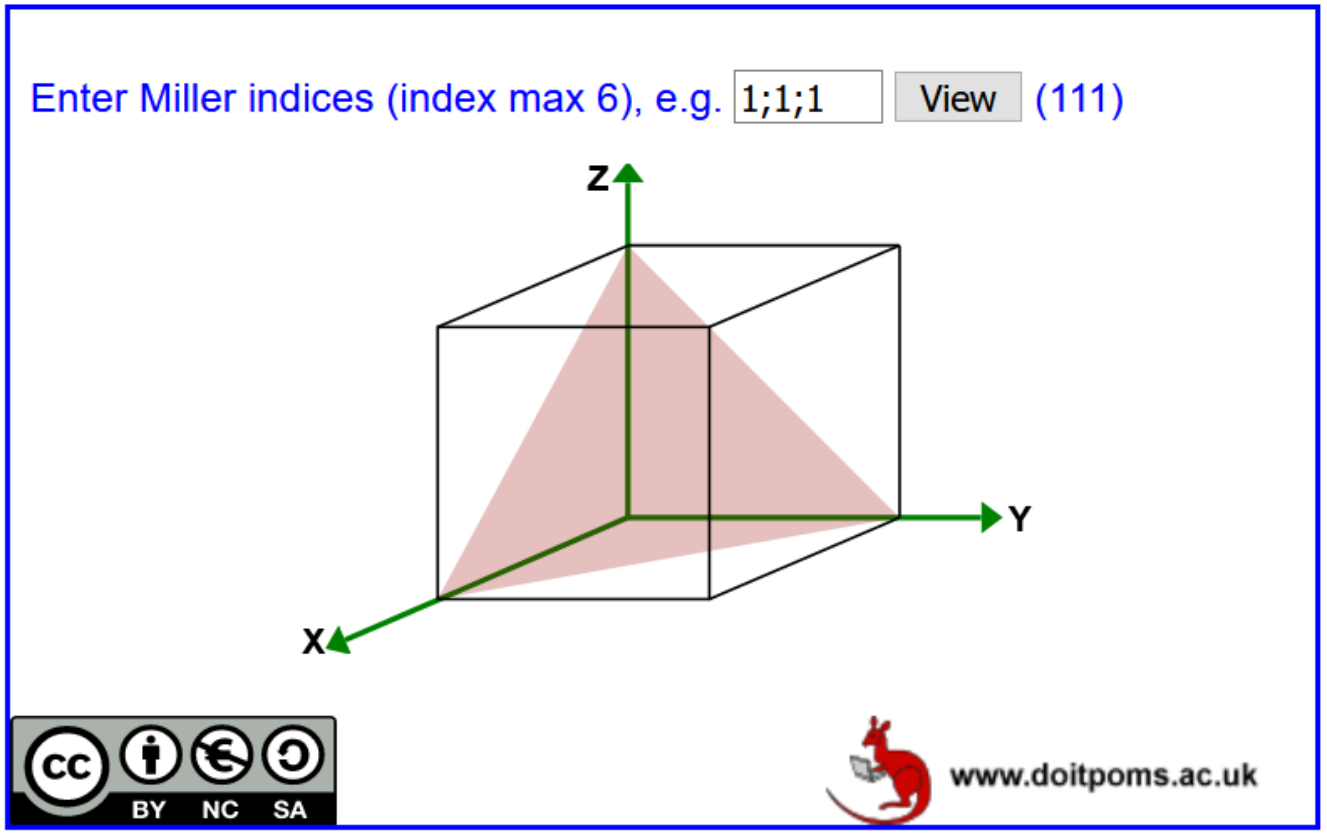
Miller Indices



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

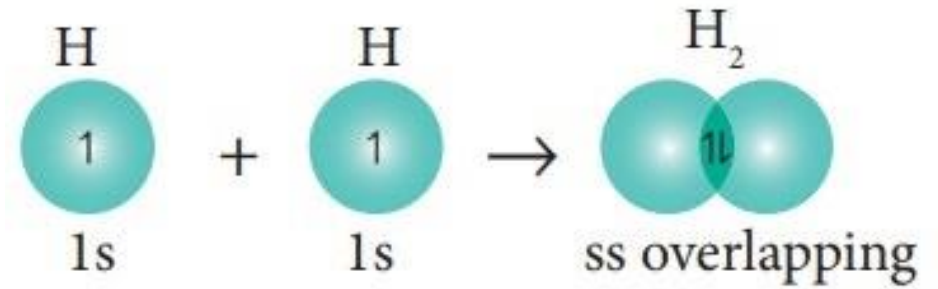


Draw your own lattice planes

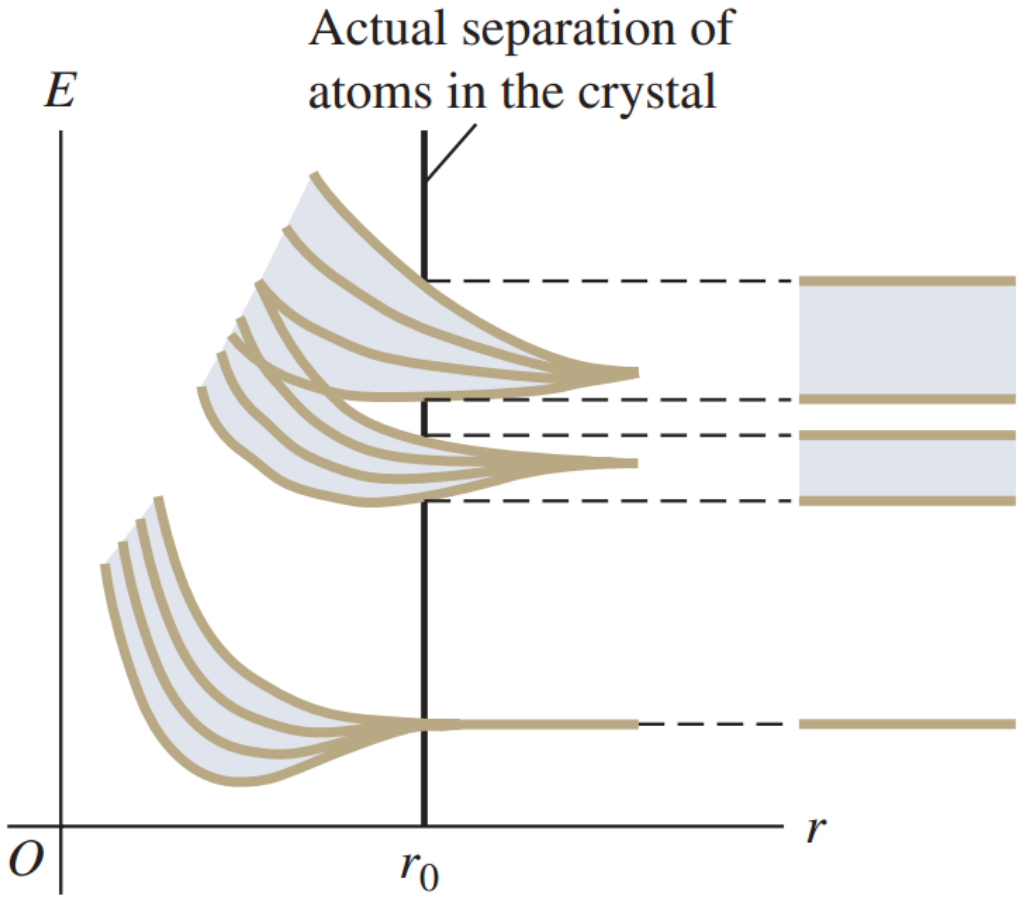


https://www.doitpoms.ac.uk/tlplib/miller_indices/lattice_draw.php

Band Theory of Solids



Formation of hydrogen molecule



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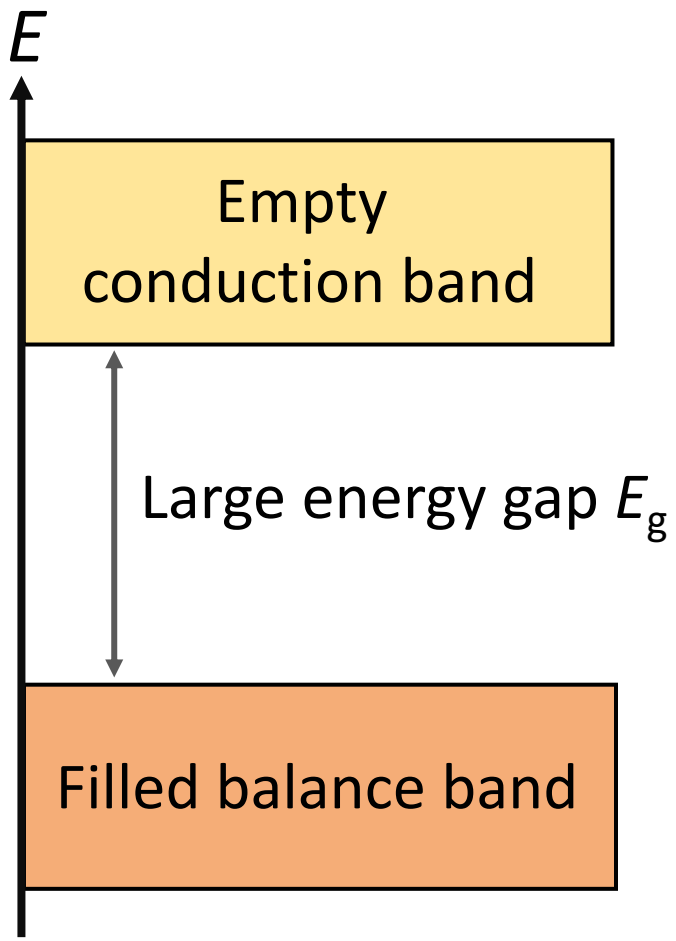
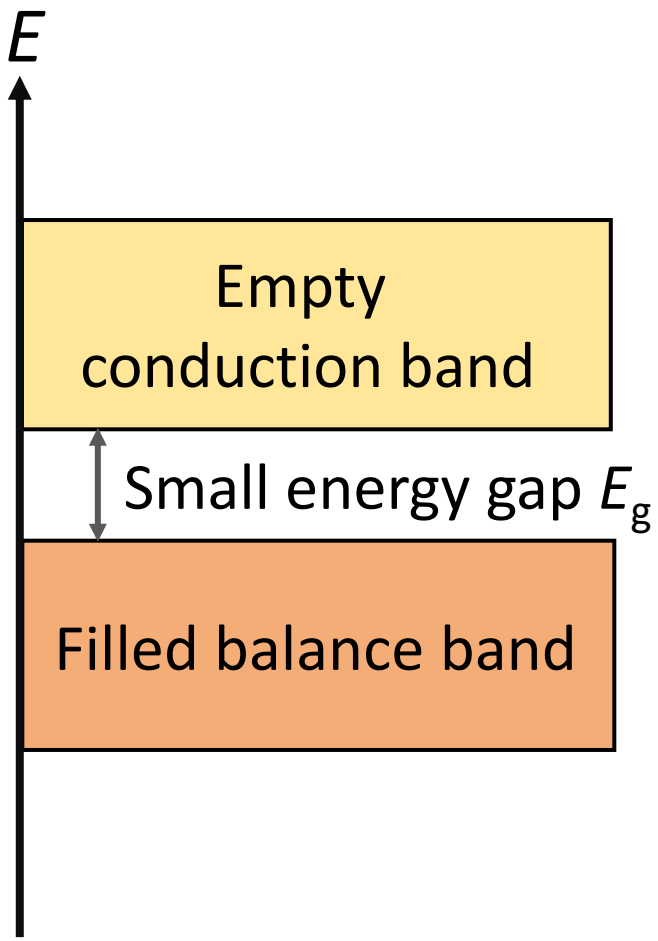
University Physics– Young, Freedman

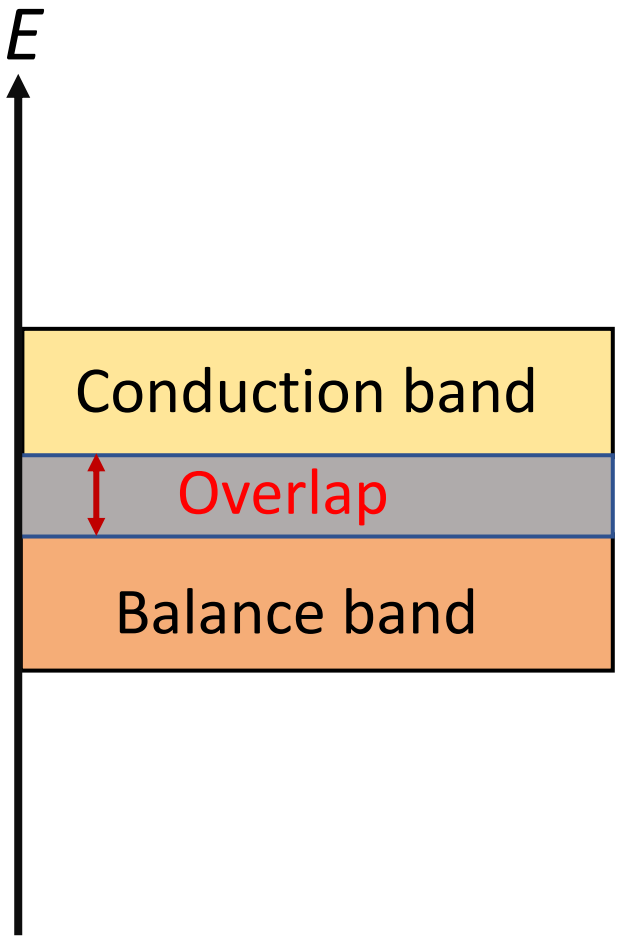
Energy Bands for Solids



Insulator

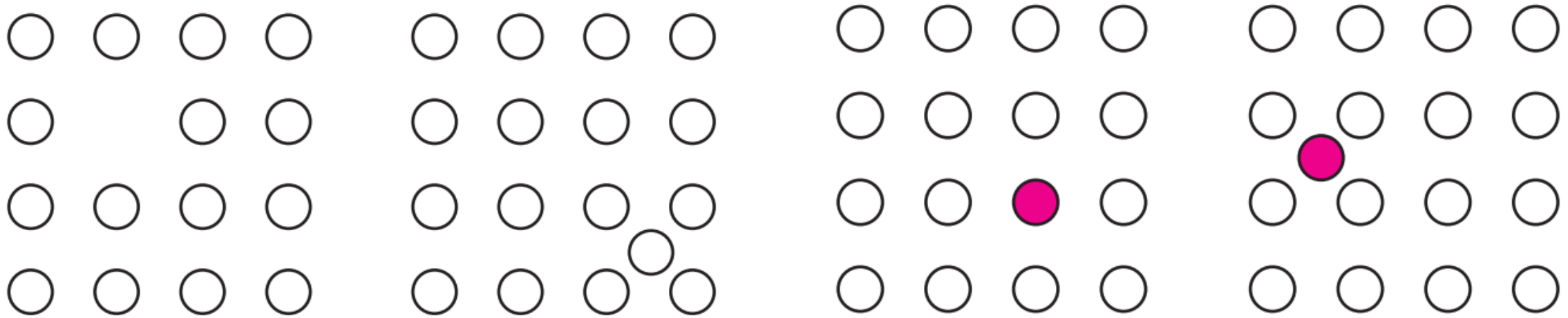


Semiconductor



Conductor

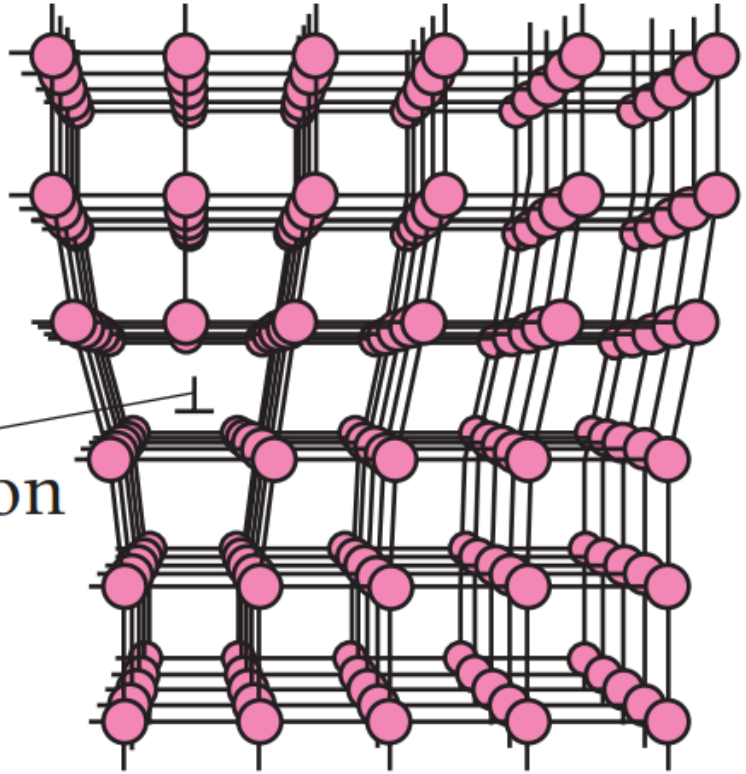
Crystal Defects

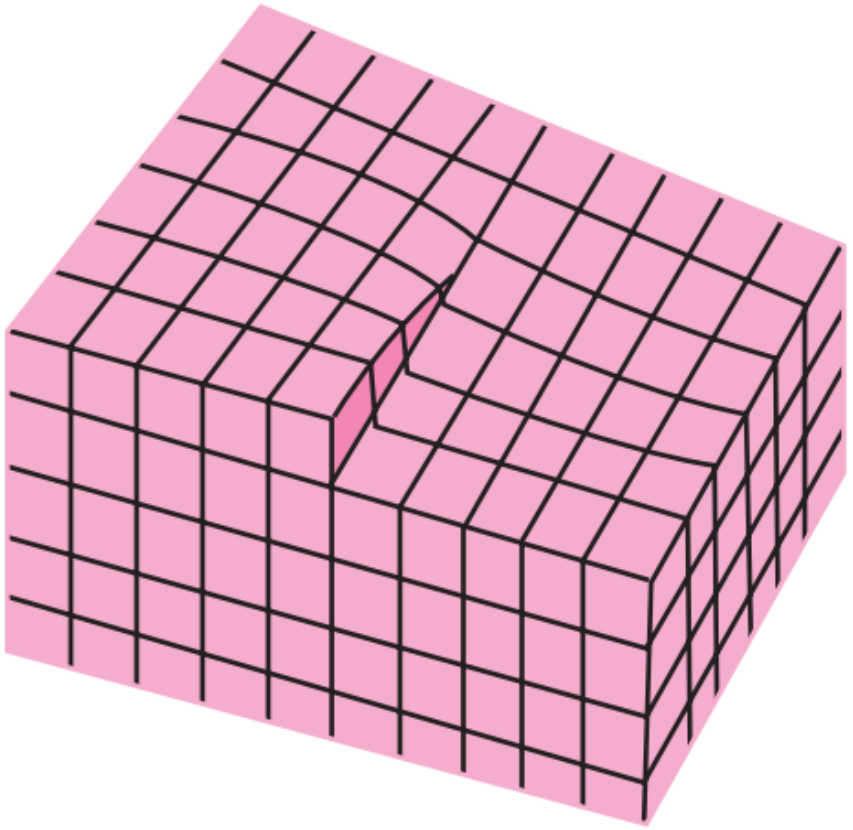


Point defects in a crystal. (*a*) Vacancy. (*b*) Interstitial. (*c*) Substitutional impurity. (*d*) Interstitial impurity.

Concepts of Modern Physics – Arthur Beiser

Crystal Defects





A screw dislocation.

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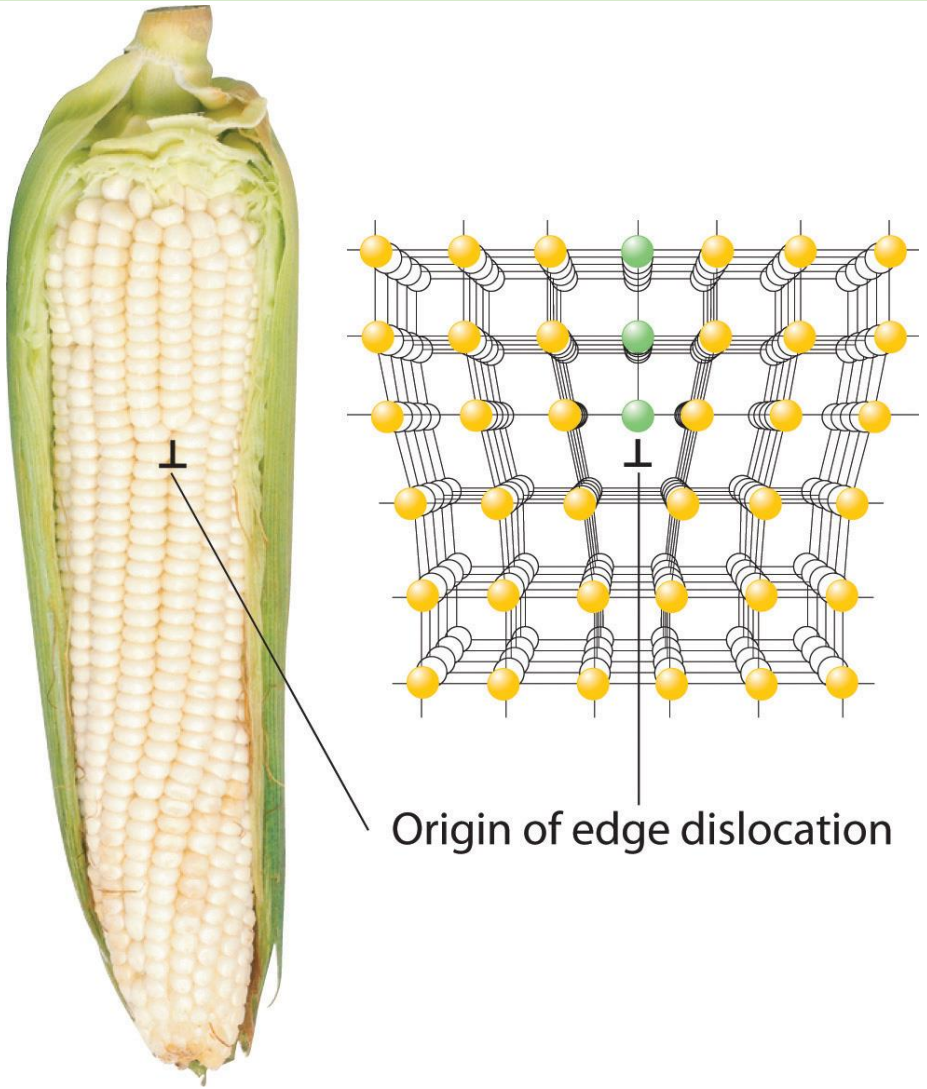
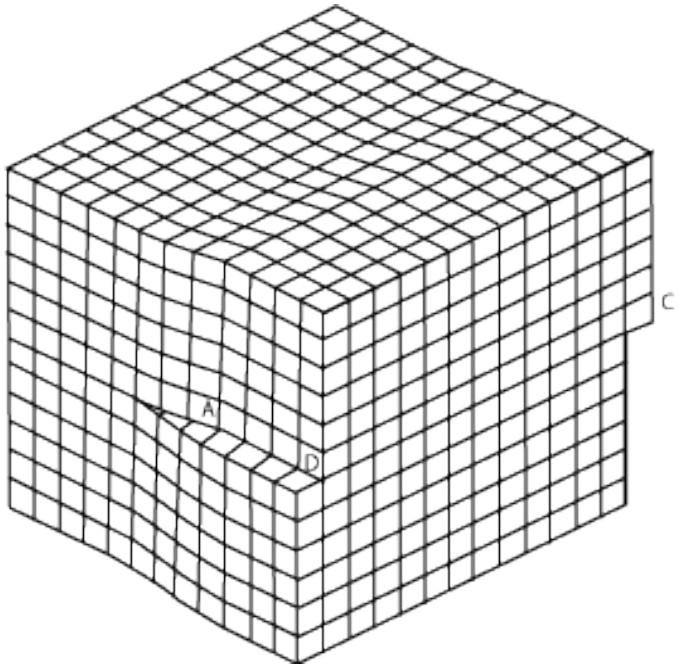
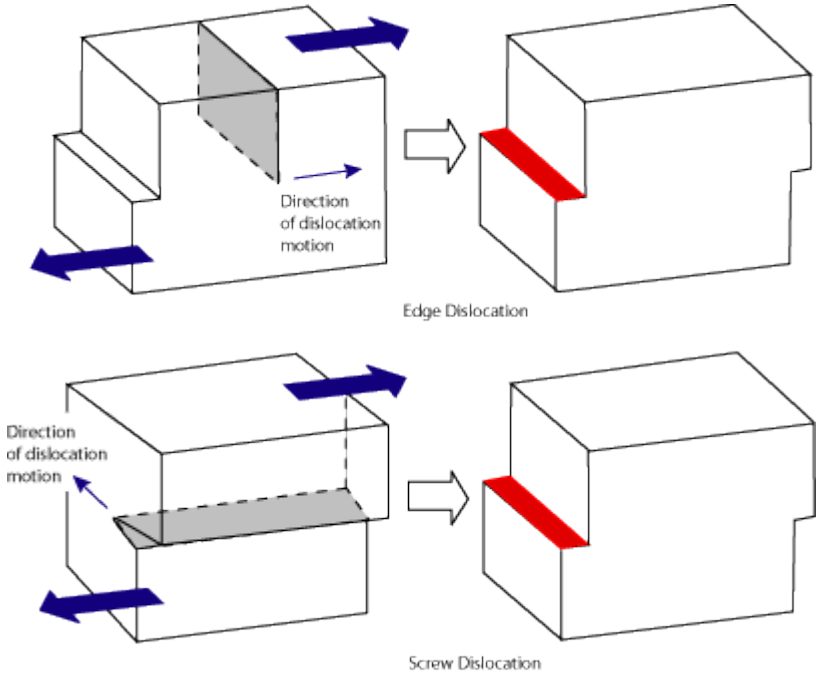
Crystal Defects



Crystal Defects





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