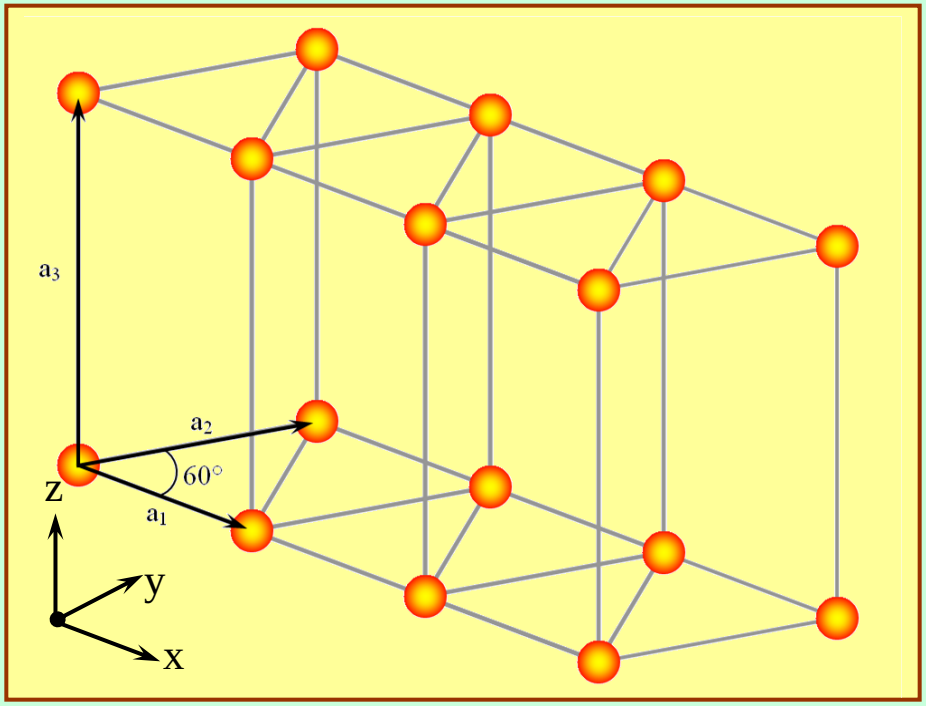

Introduction to Solid State Physics

Lecture 2

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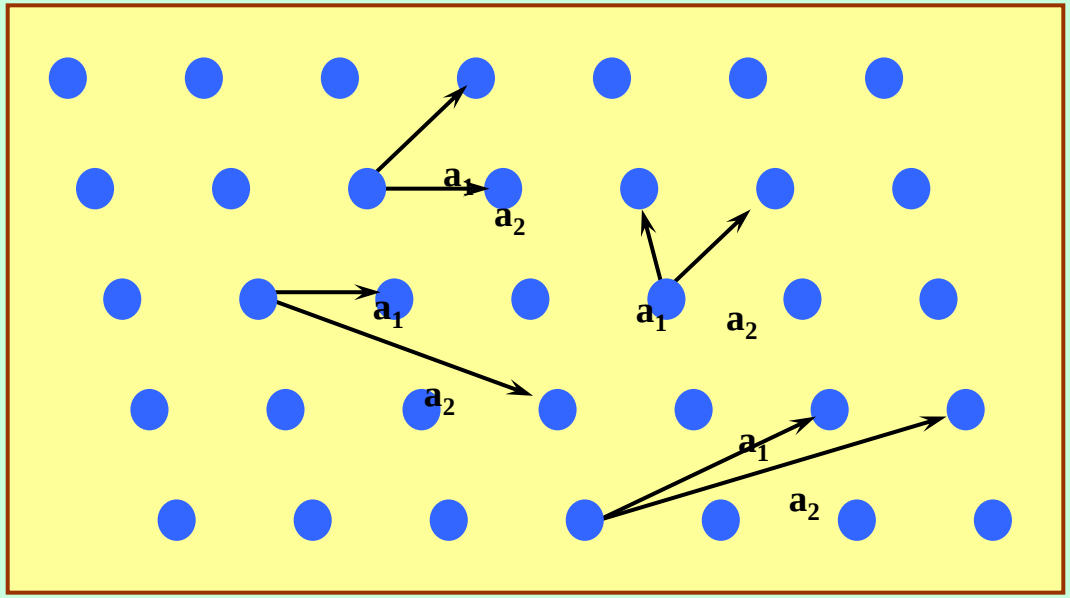
Primitive Vectors of a Bravais Lattice

By definition all Bravais lattices must be described by a set of primitive vectors $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ (in 3D). However, the choice of the set of vectors is not unique. Four choices of pairs of primitive vectors in a 2D Bravais Lattice are shown below.

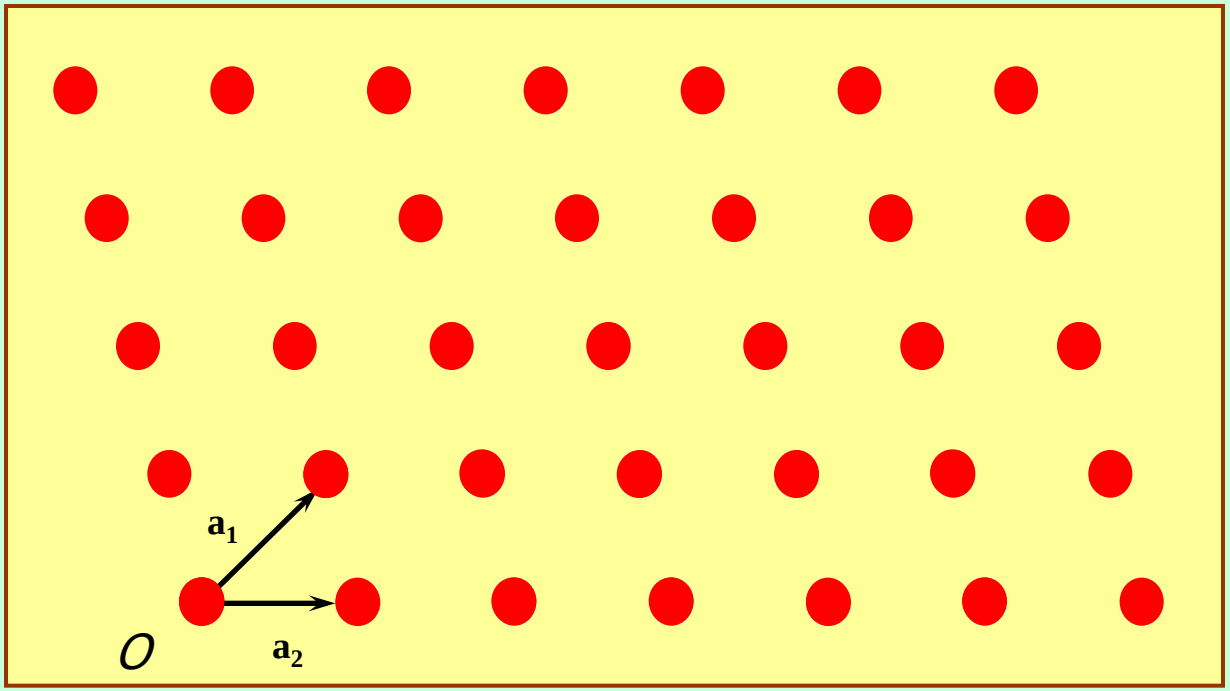
The different pairs of vectors correspond to different choices of primitive vectors in this 2D Bravais Lattice.



Primitive Vectors of a Bravais Lattice

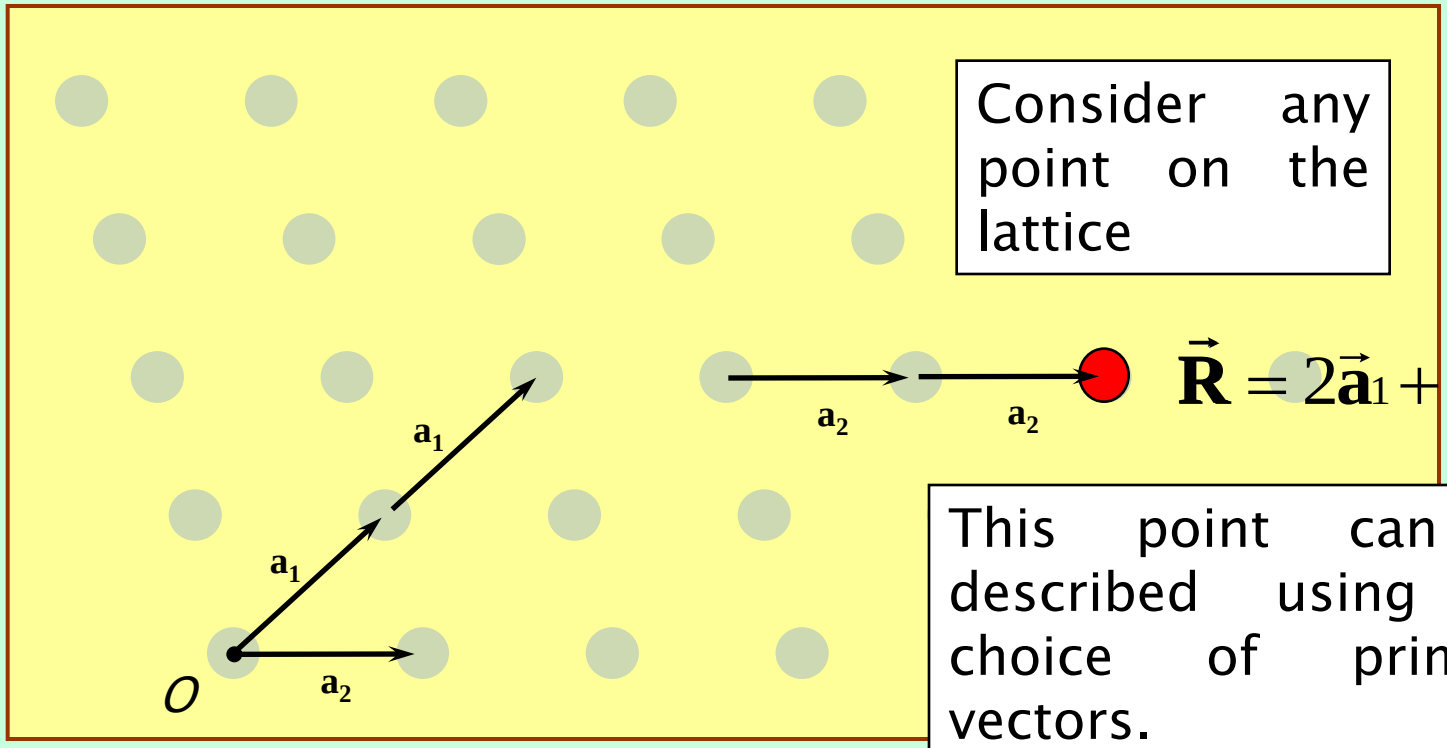
Nominate one point of the lattice to be the origin and select a set of primitive vectors.

Translating a point through combinations of these two vectors gives our original lattice.



Primitive Vectors of a Bravais Lattice

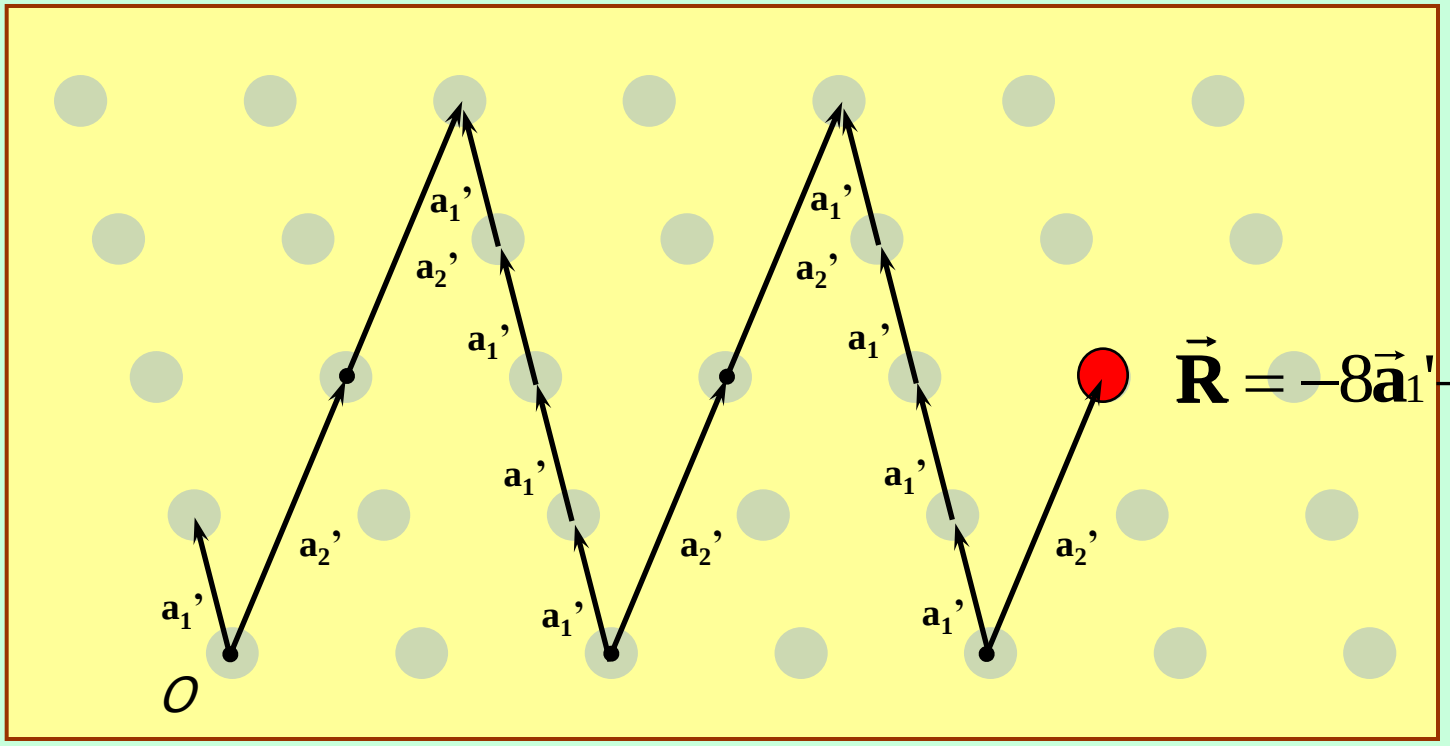
Another way of saying this is to say that every point in the lattice can be described by a linear combination of our primitive vectors.



Primitive Vectors of a Bravais Lattice

What if we had selected a different set of primitive vectors?

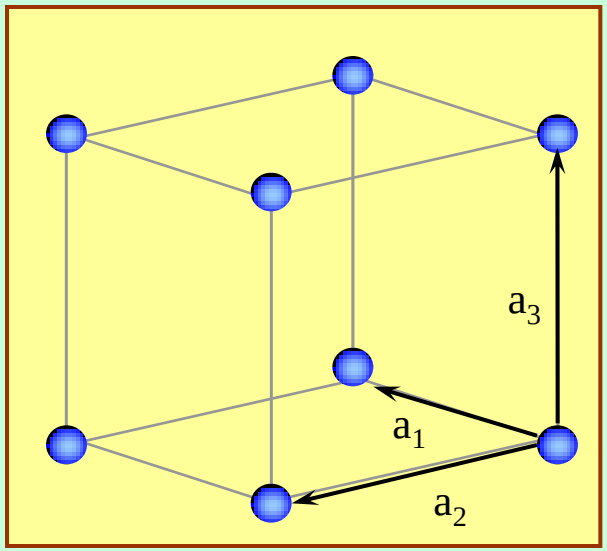
Our point can still be described by a combination of the primitive vectors. And so each choice of primitive vectors can construct the lattice.



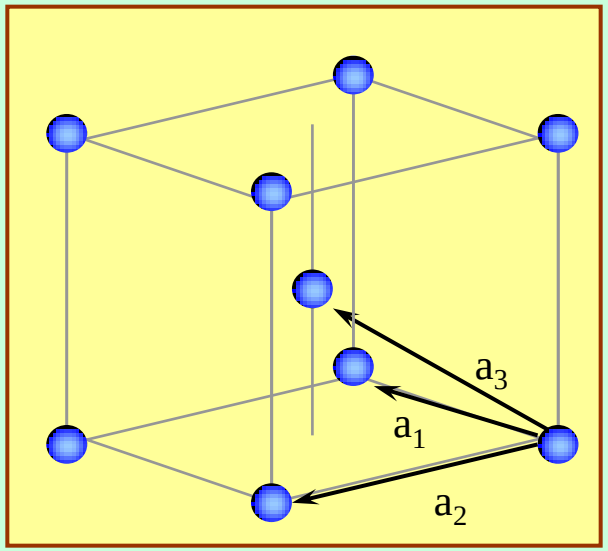
Bravais Lattice

Three most common 3D Bravais lattices:

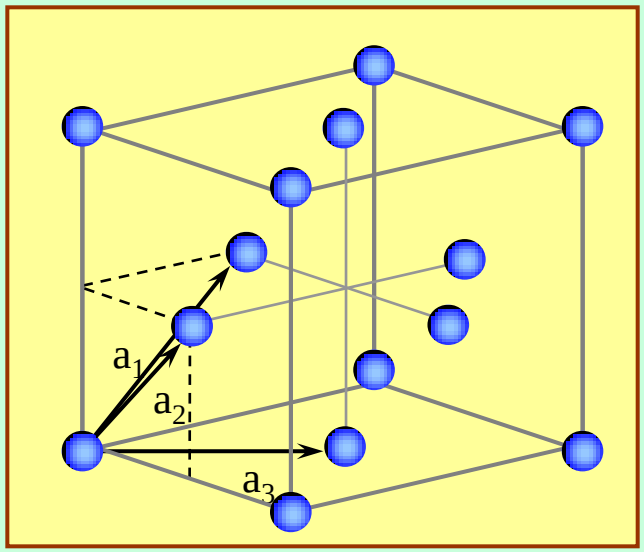
1. Simple Cubic (sc)
2. Body-Centred Cubic (bcc)
3. Face-Centred Cubic (fcc)



Simple Cubic lattice



Body-Centred Cubic lattice.



Face-Centred Cubic lattice.

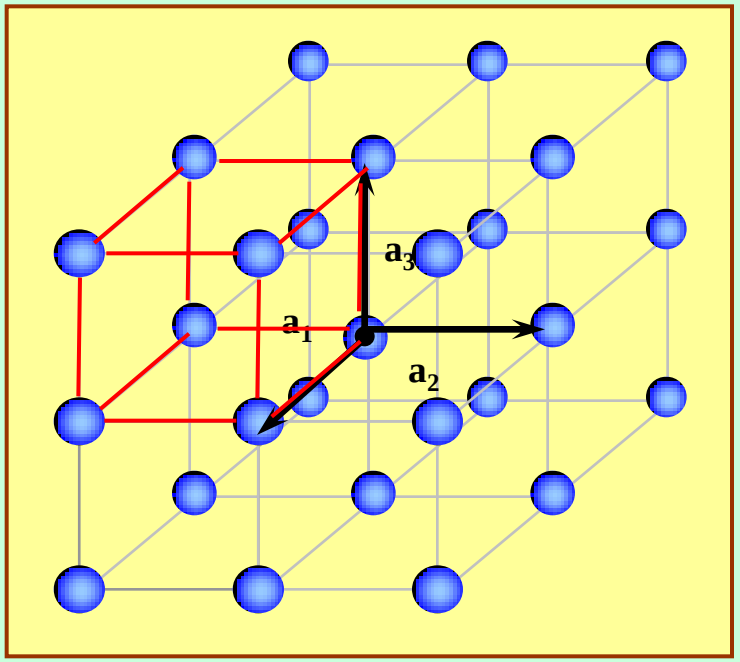
Simple Cubic (SC)

The Simple Cubic Lattice is one of the most familiar 3D Bravais lattices. It is very common but only with multi-atom basis. Crystals with single atom basis and simple cubic lattice are rarely found in nature, the alpha phase of polonium being the only known example among the elements under normal conditions.

Primitive Vectors

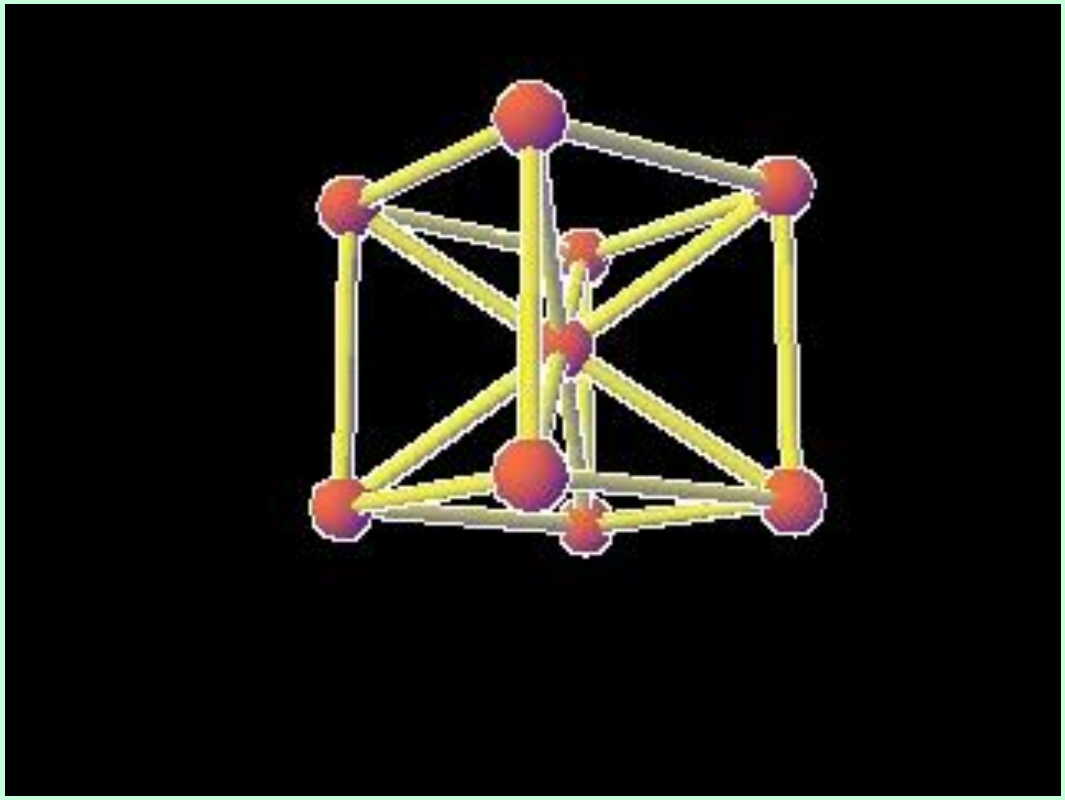
In the simple cubic structure it is easiest to take the primitive vectors to be mutually perpendicular, and with a common magnitude, a.

$$\mathbf{a}_1 = a\hat{x}\,,\quad \mathbf{a}_2 = a\hat{y}\,,\quad \mathbf{a}_3 = a\hat{z}$$



Body-Centered Cubic (BCC)

The BCC lattice is similar to the Simple Cubic with an extra point at the centre of the single cube.



Body-Centered Cubic (BCC)

Table 2.1Examples of elements with bcc structure

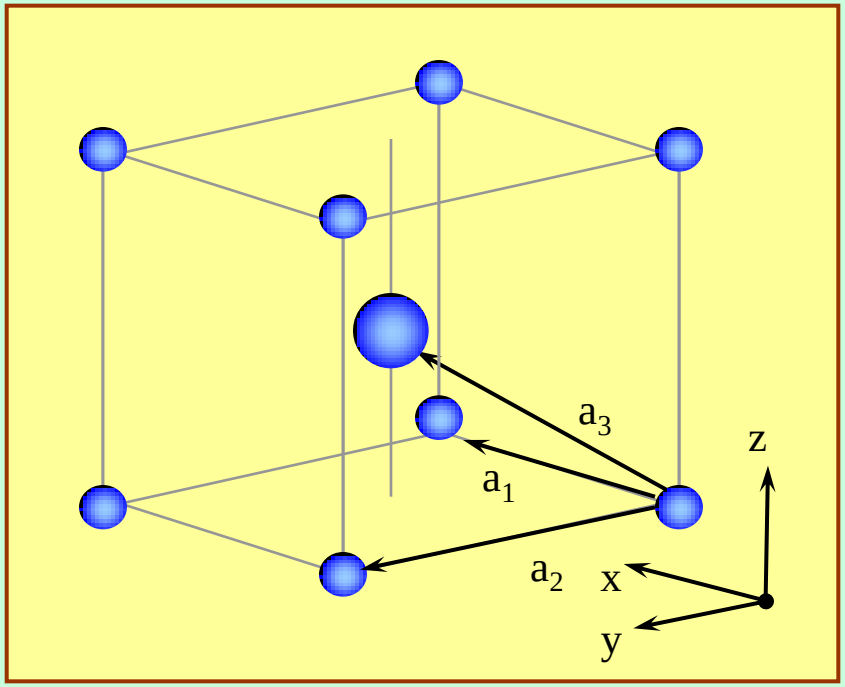
ELEMENT	a (A)	ELEMENT	a (A)	ELEMENT	a (A)
Ba	5.02	K	5.23 (5K)	Nb	3.30
Cr	2.88	Li	3.49 (78K)	Rb	5.59 (5K)
Cs	6.05 (78K)	Mo	3.15	Ta	3.31
Fe	2.87	Na	4.23 (5K)	Tl	3.88

Primitive Vectors

A particular choice of primitive vectors for the BCC is shown in the diagram.

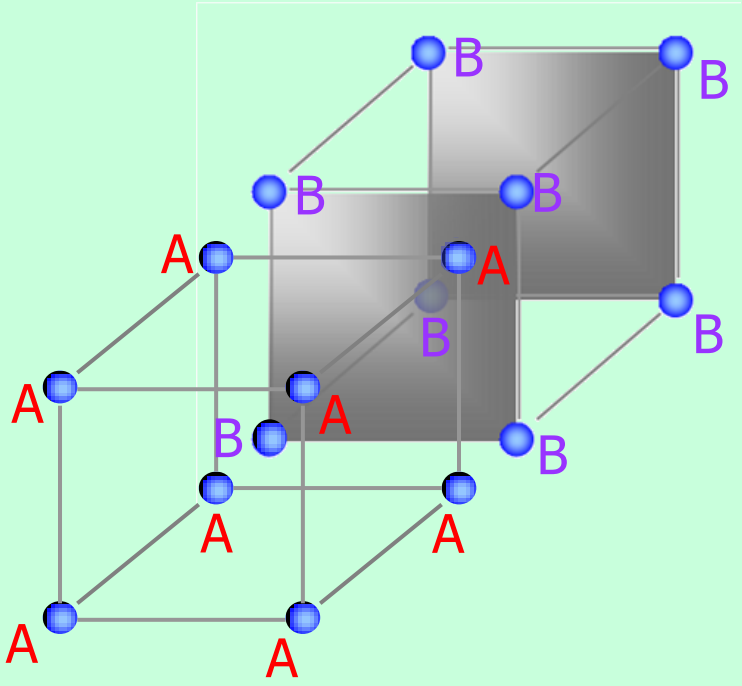
$$a_1 = a\hat{x}\ ,\ a_2 = a\hat{y}\ ,$$

$$a_3 = \frac{a}{2}\left(\hat{x}+\hat{y}+\hat{z}\right)$$



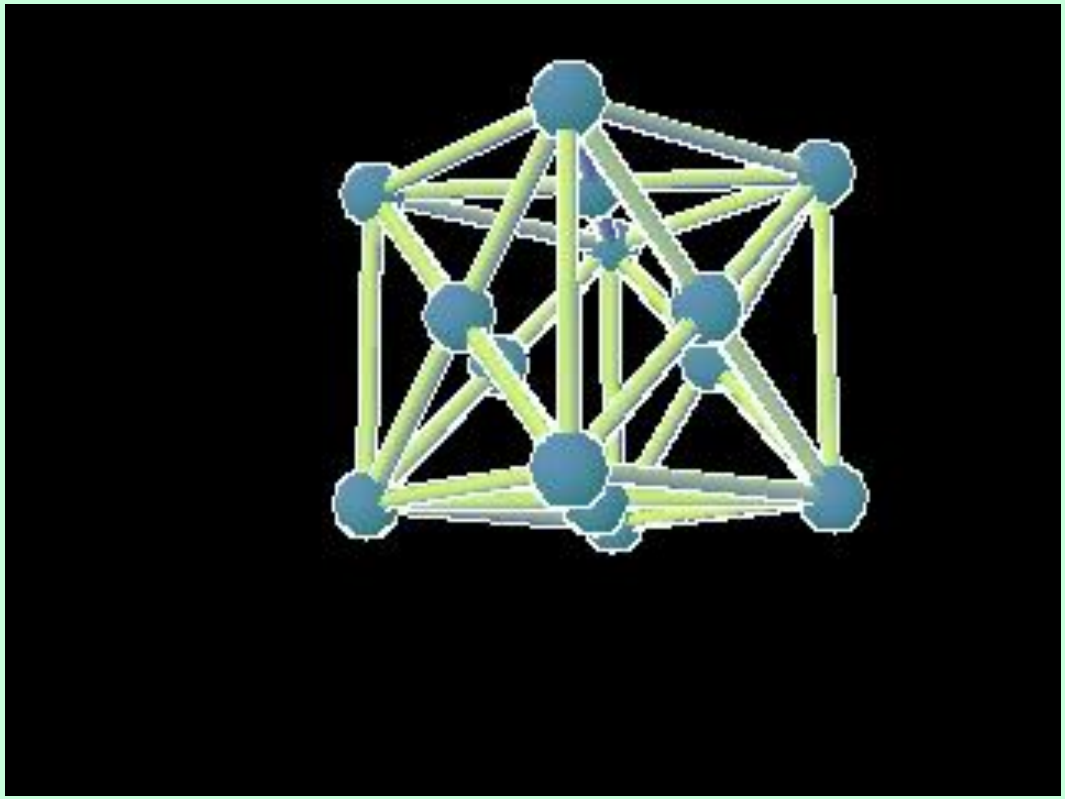
Body-Centered Cubic (BCC)

It may be difficult at first to see that the BCC lattice is in fact a Bravais lattice; the central point of the cube may be thought to be different to the corner points. However, if you consider the centre point to be the corner of a second simple cubic it becomes clear that this is the case.



Face-Centered Cubic (FCC)

The FCC lattice is again similar to the Simple Cubic. However, now there are extra points on each face of the cube.



Face-Centered Cubic (FCC)

Table 2.2 Examples of elements with fcc structure

ELEMENT	a (A)	ELEMENT	a (A)	ELEMENT	a (A)
Ar	5.26 (4.2K)	Ca	5.58	Kr	5.72 (58K)
Ag	4.09	Ce	5.16	La	5.30
Al	4.05	Cu	3.61	Ne	4.43 (4.2K)
Au	4.08	Ir	3.84	Ni	3.52

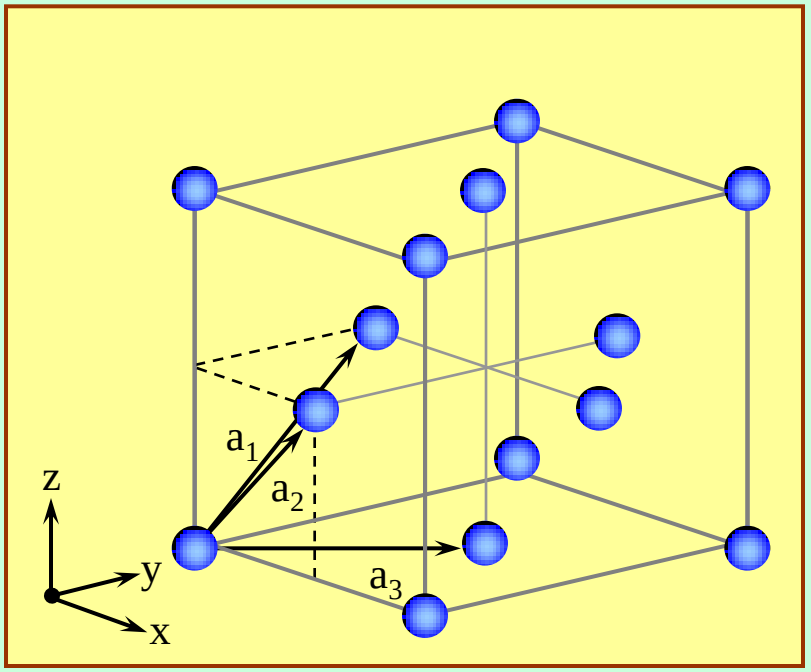
Primitive Vectors

A symmetric choice of primitive vectors for the FCC is shown in the diagram.

$$a_1 = \frac{a}{2}\left(\hat{y} + \hat{z}\right)$$

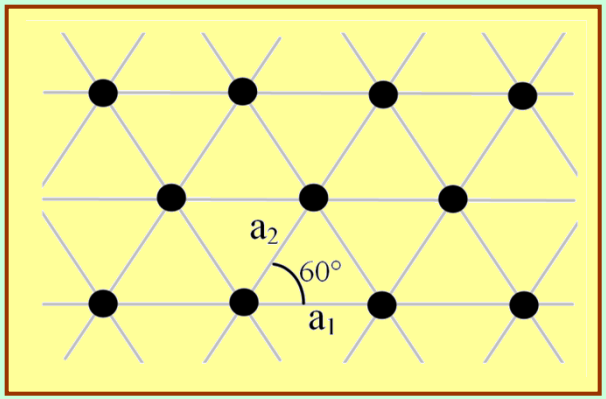
$$a_2 = \frac{a}{2}\left(\hat{z} + \hat{x}\right)$$

$$a_3 = \frac{a}{2}\left(\hat{x} + \hat{y}\right)$$



Simple Hexagonal Bravais lattice

This is an example of a non-cubic Bravais lattice. It consists of 2D triangular nets stacked directly above each other.
Since the structure is hexagonal all triangles must be equilateral.

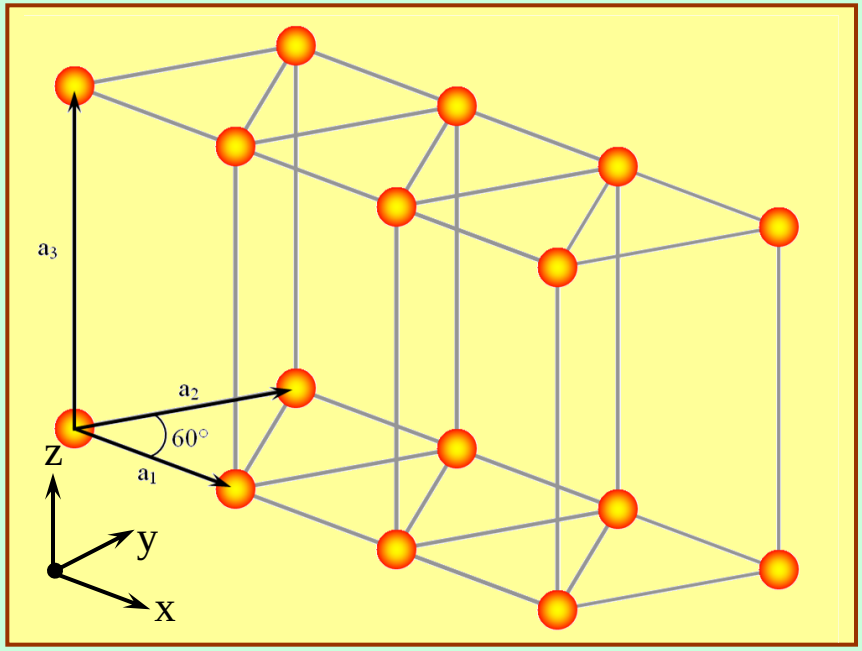


Primitive Vectors

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

$$\vec{\mathbf{a}}_2 = \frac{a}{2}\vec{\mathbf{x}} + \frac{\sqrt{3}}{2}\vec{\mathbf{y}}$$

$$\vec{\mathbf{a}}_3 = c\vec{\mathbf{z}}$$



Coordination Number

The points in a Bravais lattice that are closest to a given point are called its nearest neighbors.

Since Bravais lattices are periodic, each point in the lattice has the same number of nearest neighbors. This number is a property of the lattice and is called its coordination number.

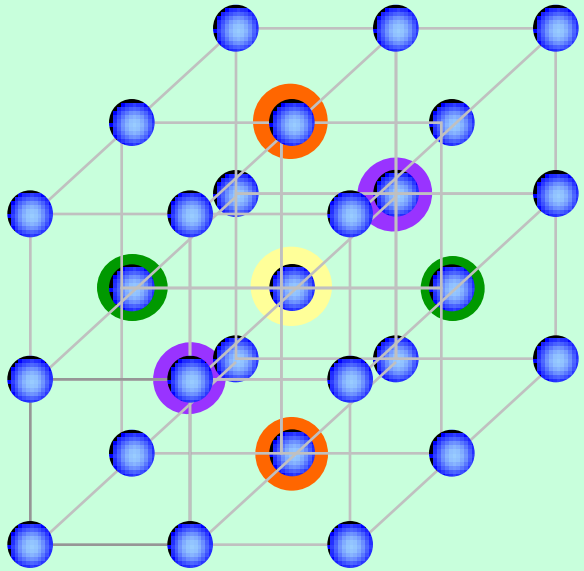
Convince yourselves of the following:

Bravais Lattice	Coordination Number
Simple Cubic	6
bcc	8
fcc	12

Coordination Number

Example: The coordination number of the simple cubic lattice is 6 due to the six nearest neighbours of each point.

Consider a point of the simple cubic lattice. It nearest neighbours are located…



2 in the x-direction

2 in the y-direction

2 in the z-direction

Primitive Unit Cell

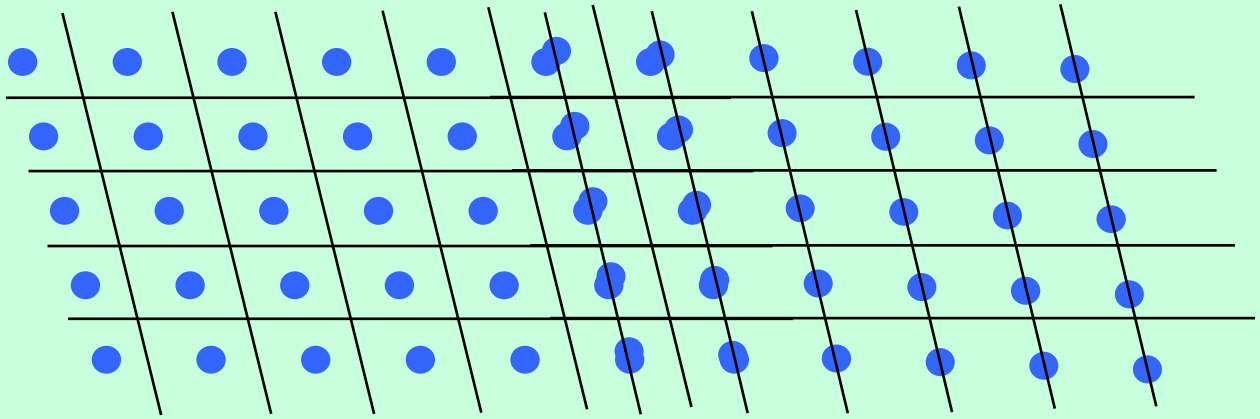
The **primitive unit cell** is the volume that, when translated through **all the vectors** in a Bravais lattice just fills all space without overlapping or leaving voids. Here the word "all" means: pick any three Bravais vectors of the infinite choice and they will do the job.

The primitive unit cell can be defined mathematically as the set of all points of the form;

$$\mathbf{r} = x_1\mathbf{a_1} + x_2\mathbf{a_2} + x_3\mathbf{a_3}$$

where $\mathbf{a_1}$, $\mathbf{a_2}$ and $\mathbf{a_3}$ are a set of primitive vectors and possibilities for x_1 ,x_2 and x_3 range continuously between 0 and 1.

Primitive Unit Cell



Each primitive unit cell contains just one point of the Bravais lattice even if it is positioned that there are points on its surface. In either case, it is still one point of Bravais lattice assigned to each cell

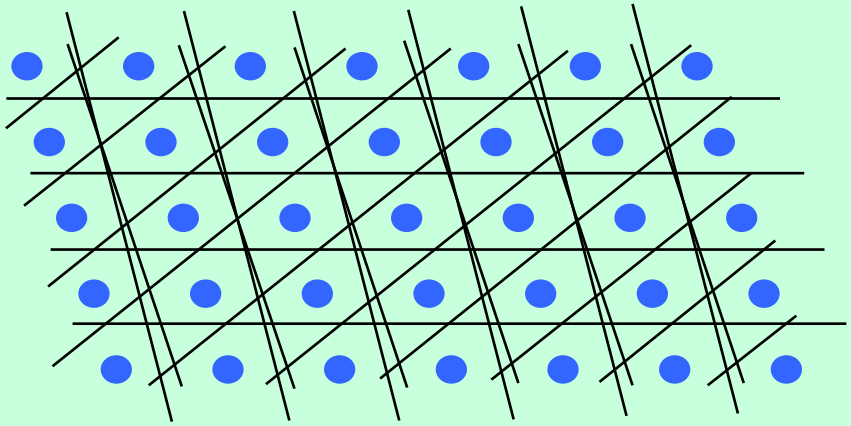
Therefore, the volume V of the primitive unit cell is given by

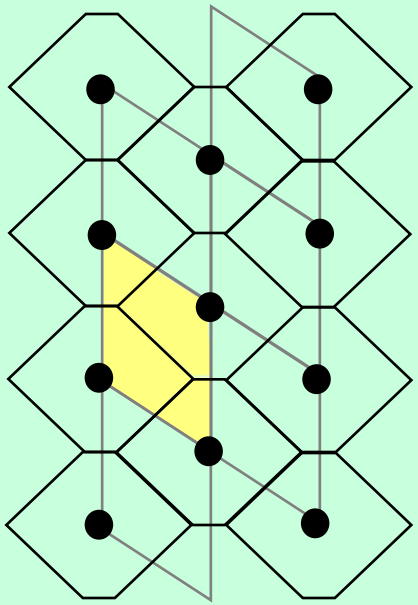
$$V = 1/n$$

where n is the density of points.

Primitive Unit Cell

Since there is no unique choice of primitive vectors there is no unique way of choosing the primitive unit cell.





The volume of each choice of primitive cell must be the same. One can re-assemble a primitive cell into another cell. This is achieved by cutting the cell into segments and translating them by linear combinations of primitive vectors.

Primitive Unit Cell

One problem with using the primitive unit cell to describe a Bravais lattice is that it doesn't display the full symmetry of the lattice.

Unit Cell

There are two ways to get around the problem of symmetry when choosing a unit cell;

1. Wigner-Seitz primitive cell about a lattice point is the region of space that is closer to that point than to any other lattice point.

2. Conventional unit cell or non-primitive unit cell. This is the unit cell that fills up all the space without any overlapping when translated through some subset of the vectors of a Bravais lattice. The conventional cell is generally bigger than the primitive cell (i.e. generally has more than one lattice point per cell). Dimensions specifying the size of the unit cell are called lattice constants.

Wigner-Seitz Primitive Cell

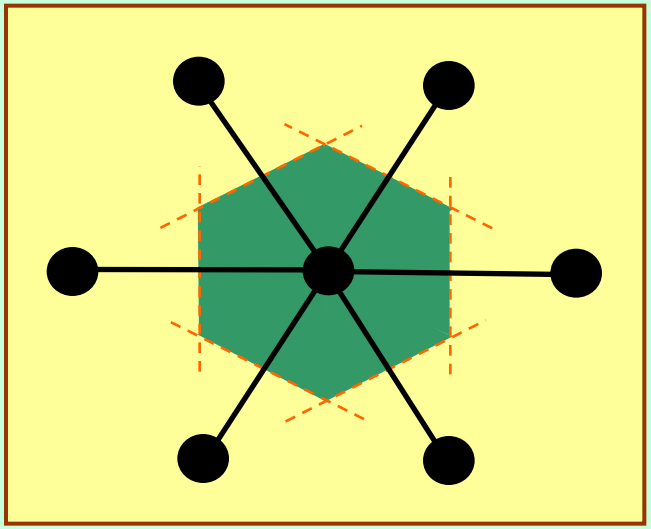
Constructing the Wigner-Seitz Primitive cell

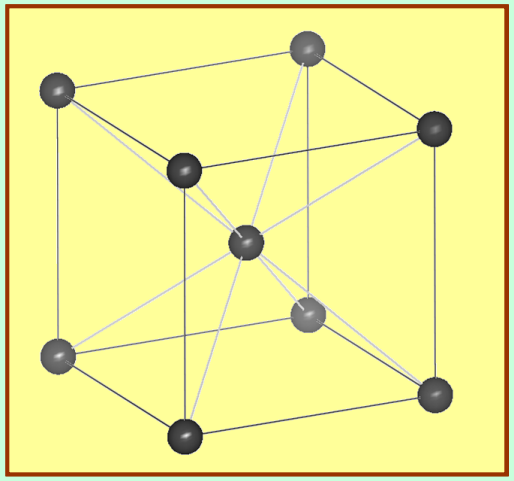
Pick a point in the lattice.

Draw lines to connect this point to its nearest neighbors

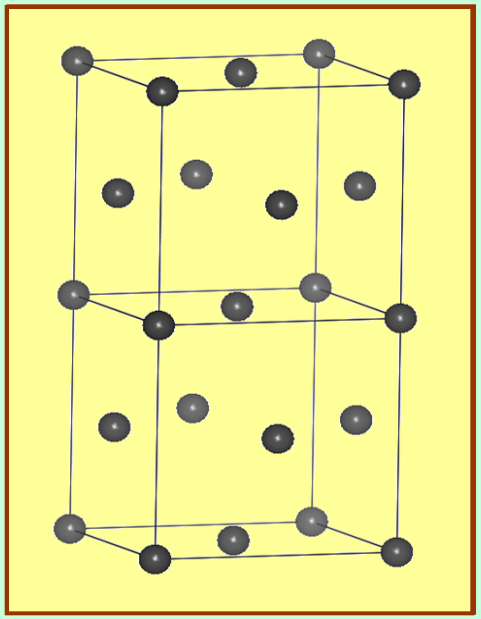
Bisect these lines and join up the bisectors.

The area enclosed is the Wigner-Seitz Primitive cell





Wigner-Seitz of bcc lattice



Wigner-Seitz of fcc lattice

Conventional unit Cell

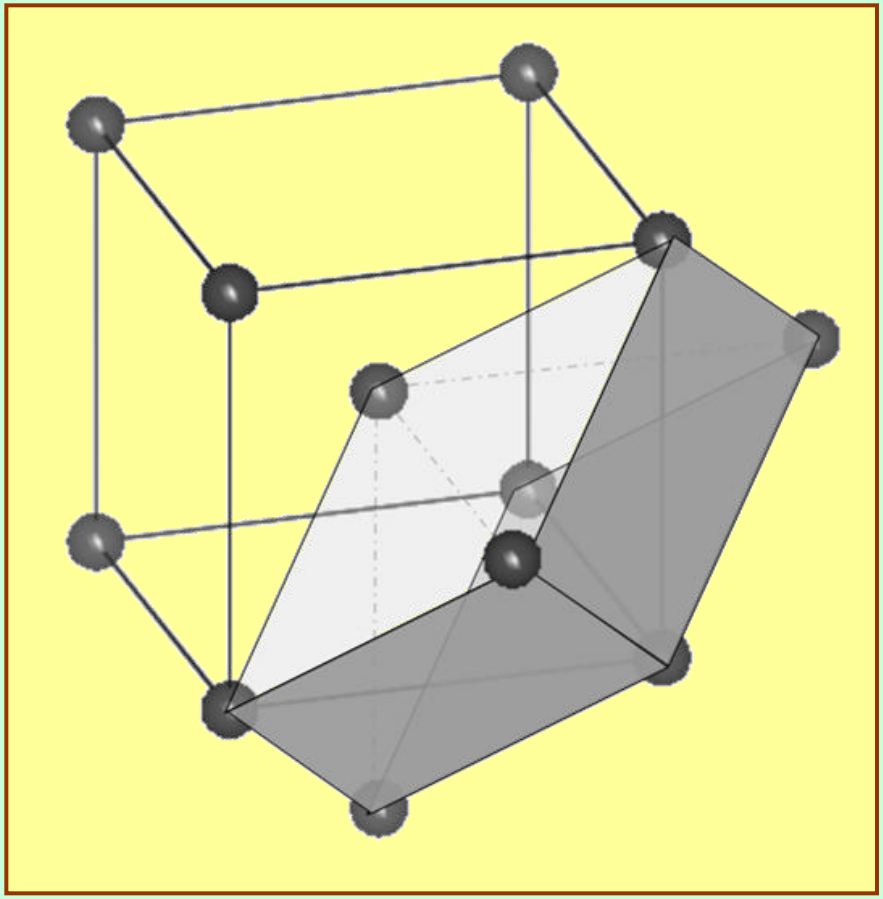
Body Centred Cubic

Primitive and conventional unit cells are shown for the case of the bcc lattice.

The conventional cell is the large cube.

The primitive cell is shaded.

The total volume of the conventional cell is **twice** that of the primitive cell, since it contains **two** points of the lattice



Conventional unit Cell

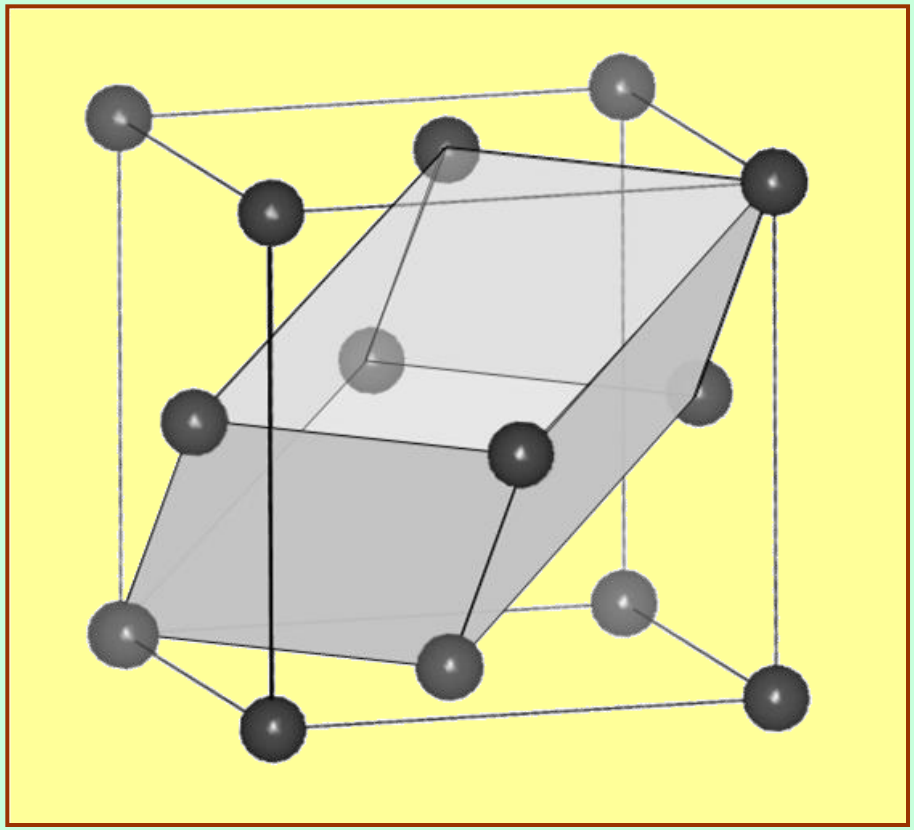
Face Centred Cubic

Primitive and conventional unit cells are shown for the case of the fcc lattice.

The conventional cell is the large cube.

The primitive cell is the shaded figure with six parallelogram faces.

The volume of the conventional cell is **four** times that of the primitive cell, since it contains **four** points of the lattice.

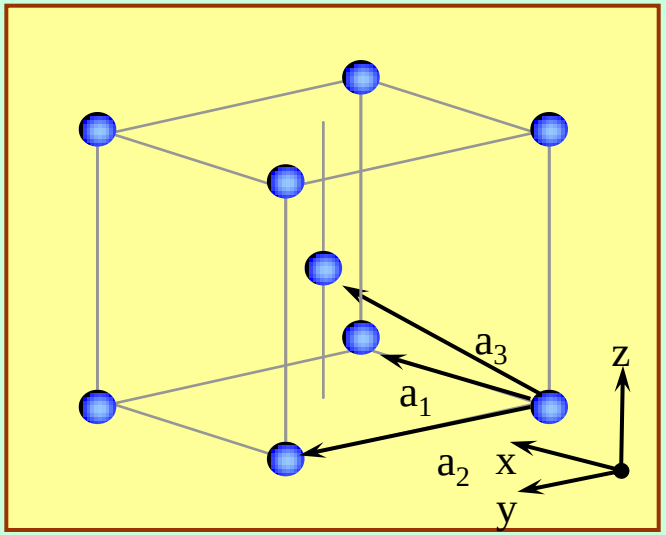


Exercise

In an earlier slide you were given one possibility for the primitive vectors of a BCC lattice.

$$a_1 = a\hat{x}\ ,\ a_2 = a\hat{y}\ ,$$

$$a_3 = \frac{a}{2}\left(\hat{x} + \hat{y} + \hat{z}\right)$$



These vectors are not symmetric. Construct a set of symmetric primitive vectors for the BCC lattice.

[Hint: You may wish to consider more than one cubic cell.]

Problems/Questions?

- What is a Primitive vector?
- What is the difference between a primitive cell and a conventional unit cell?
- Can you construct a Wigner-Seitz primitive cell?
- Can you visualise BCC and FCC lattice structure?
  - If not visit www.dawgsdk.org/crystal/en/library
  - Or download a viewer; http://demonstrations.wolfram.com/crystalviewer

I would urge you to know the answers to these questions before next time.

Good resources

- Solid State Physics ~ Ashcroft, Ch. 4
- Introduction to Solid State Physics ~ Kittel, Ch. 1
- The Physics and Chemistry of Solids ~ Elliott, Ch. 2
- Solid State Physics ~ Hook & Hall, Ch. 1