

Handout 4

Lattices in 1D, 2D, and 3D

In this lecture you will learn:

- Bravais lattices
- Primitive lattice vectors
- Unit cells and primitive cells
- Lattices with basis and basis vectors



August Bravais (1811-1863)

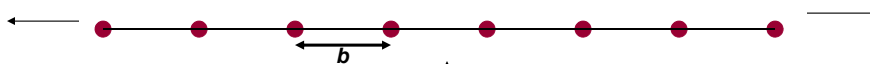
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Bravais Lattice

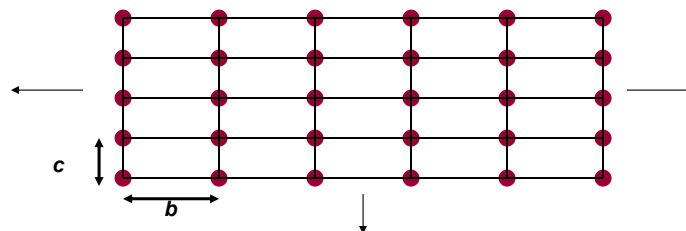
A fundamental concept in the description of crystalline solids is that of a “Bravais lattice”. A Bravais lattice is an infinite arrangement of points (or atoms) in space that has the following property:

The lattice looks exactly the same when viewed from any lattice point

A 1D Bravais lattice:



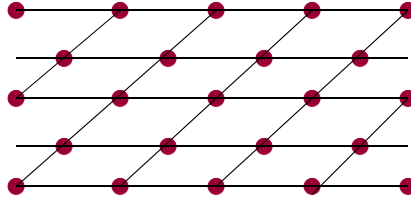
A 2D Bravais lattice:



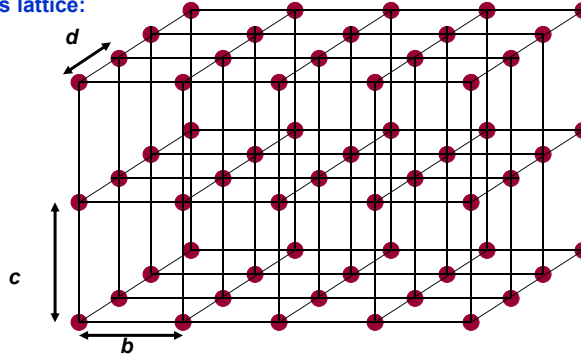
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Bravais Lattice

A 2D Bravais lattice:



A 3D Bravais lattice:



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Bravais Lattice

A Bravais lattice has the following property:

The position vector of all points (or atoms) in the lattice can be written as follows:

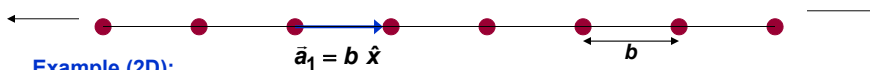
$$\begin{aligned}
 \text{1D} \quad & \vec{R} = n \vec{a}_1 \\
 \text{2D} \quad & \vec{R} = n \vec{a}_1 + m \vec{a}_2 \\
 \text{3D} \quad & \vec{R} = n \vec{a}_1 + m \vec{a}_2 + p \vec{a}_3
 \end{aligned}$$

Where $n, m, p = 0, \pm 1, \pm 2, \pm 3, \dots$

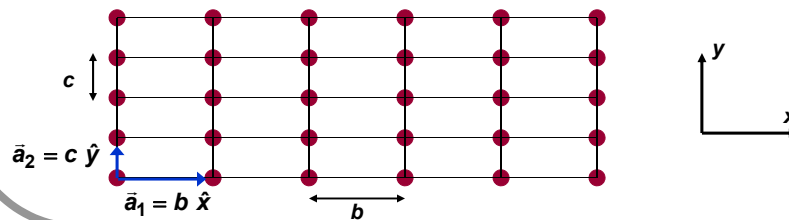
And the vectors, \vec{a}_1, \vec{a}_2 , and \vec{a}_3

are called the "primitive lattice vectors" and are said to span the lattice. These vectors are not parallel.

Example (1D):



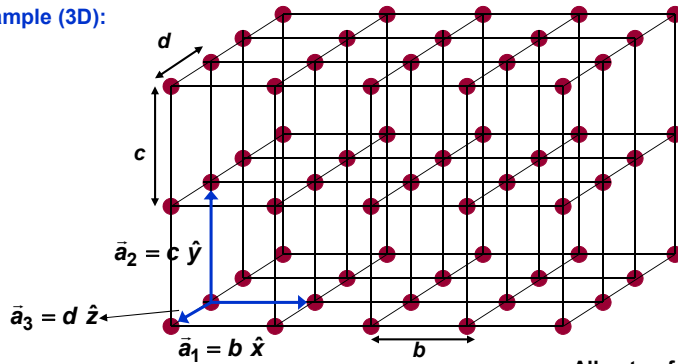
Example (2D):



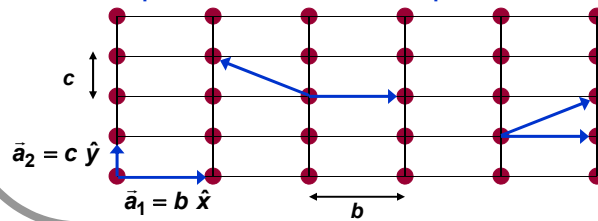
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Bravais Lattice

Example (3D):



The choice of primitive vectors is NOT unique:

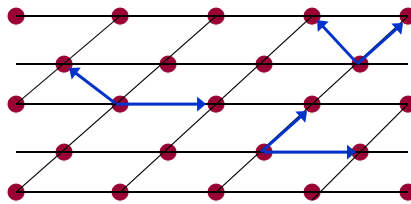


All sets of primitive vectors shown will work for the 2D lattice

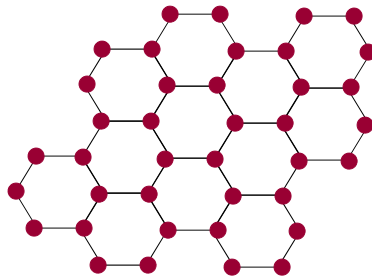
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Bravais Lattice

Example (2D):



All lattices are not Bravais lattices:

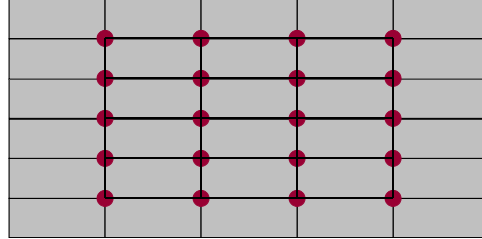
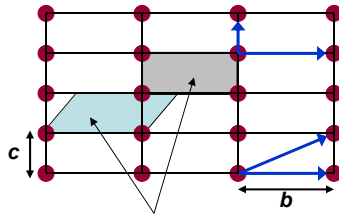


The honeycomb lattice

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The Primitive Cell

- A primitive cell of a Bravais lattice is the smallest region which when translated by all different lattice vectors can “tile” or “cover” the entire lattice without overlapping



Two different choices of primitive cell

Tiling of the lattice by the primitive cell

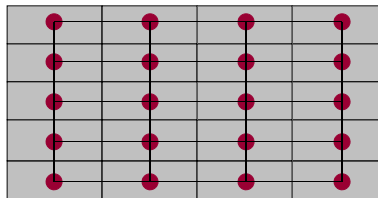
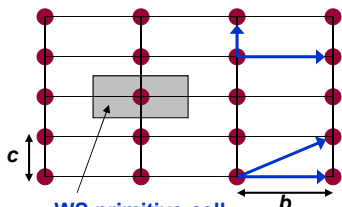
- The primitive cell is not unique
- The volume (3D), area (2D), or length (1D) of a primitive cell can be given in terms of the primitive vectors, and is independent of the choice of the primitive vectors or of the primitive cells

1D	$\Omega_1 = \bar{a}_1 $	}	Example, for the 2D lattice above:	
2D	$\Omega_2 = \bar{a}_1 \times \bar{a}_2 $		$\bar{a}_1 = b \hat{x}$ $\bar{a}_2 = c \hat{y}$	or $\bar{a}_1 = b \hat{x}$ $\bar{a}_2 = b \hat{x} + c \hat{y}$
3D	$\Omega_3 = \bar{a}_1 \cdot (\bar{a}_2 \times \bar{a}_3) $		$\Omega_2 = \bar{a}_1 \times \bar{a}_2 = bc$	$\Omega_2 = \bar{a}_1 \times \bar{a}_2 = bc$

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The Wigner-Seitz Primitive Cell

- The Wigner-Seitz (WS) primitive cell of a Bravais lattice is a special kind of a primitive cell and consists of region in space around a lattice point that consists of all points in space that are closer to this lattice point than to any other lattice point



WS primitive cell

Tiling of the lattice by the WS primitive cell

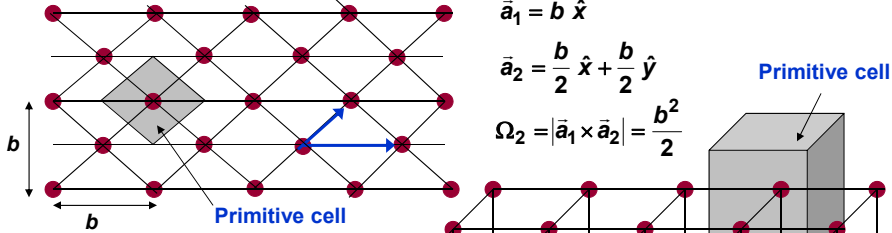
- The Wigner-Seitz primitive cell is unique
- The volume (3D), area (2D), or length (1D) of a WS primitive cell can be given in terms of the primitive vectors, and is independent of the choice of the primitive vectors

1D	$\Omega_1 = \bar{a}_1 $	}	Example, for the 2D lattice above:	
2D	$\Omega_2 = \bar{a}_1 \times \bar{a}_2 $		$\bar{a}_1 = b \hat{x}$ $\bar{a}_2 = c \hat{y}$	or $\bar{a}_1 = b \hat{x}$ $\bar{a}_2 = b \hat{x} + c \hat{y}$
3D	$\Omega_3 = \bar{a}_1 \cdot (\bar{a}_2 \times \bar{a}_3) $		$\Omega_2 = \bar{a}_1 \times \bar{a}_2 = bc$	$\Omega_2 = \bar{a}_1 \times \bar{a}_2 = bc$

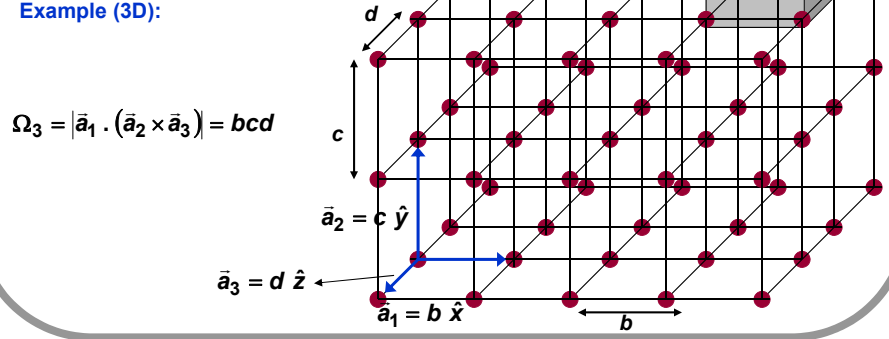
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Wigner-Seitz Primitive Cell

Example (2D):



Example (3D):

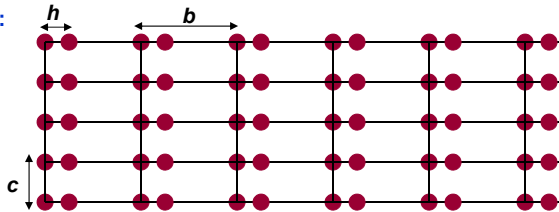


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Lattice with a Basis

Consider the following lattice:

- Clearly it is not a Bravais lattice (in a Bravais lattice, the lattice must look exactly the same when viewed from any lattice point)

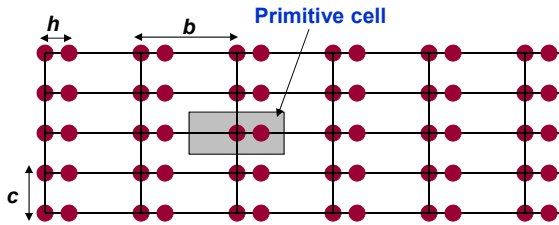


- It can be thought of as a Bravais lattice with a basis consisting of more than just one atom per lattice point – two atoms in this case. So associated with each point of the underlying Bravais lattice there are two atoms. Consequently, each primitive cell of the underlying Bravais lattice also has two atoms

- The location of all the basis atoms, with respect to the underlying Bravais lattice point, within one primitive cell are given by the **basis vectors**:

$$\bar{d}_1 = 0$$

$$\bar{d}_2 = h \hat{x}$$

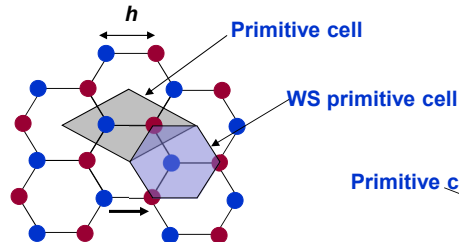


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Lattice with a Basis

Consider the Honeycomb lattice:

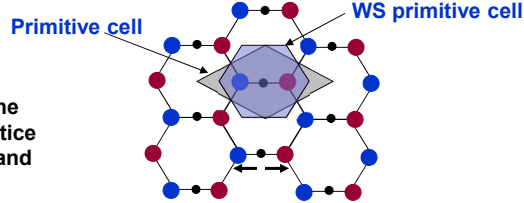
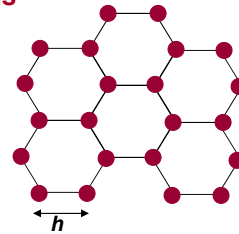
It is not a Bravais lattice, but it can be considered a Bravais lattice with a two-atom basis



I can take the "blue" atoms to be the points of the underlying Bravais lattice that has a two-atom basis - "blue" and "red" - with basis vectors:

$$\vec{d}_1 = 0 \quad \vec{d}_2 = h \hat{x}$$

Note: "red" and "blue" color coding is only for illustrative purposes. All atoms are the same.



Or I can take the small "black" points to be the underlying Bravais lattice that has a two-atom basis - "blue" and "red" - with basis vectors:

$$\vec{d}_1 = -\frac{h}{2} \hat{x} \quad \vec{d}_2 = \frac{h}{2} \hat{x}$$

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Lattice with a Basis

Now consider a lattice made up of two different atoms: "red" and "black", as shown

- It is clearly not a Bravais lattice since two different types of atoms occupy lattice positions
- The lattice defined by the "red" atoms can be taken as the underlying Bravais lattice that has a two-atom basis: one "red" and one "black"

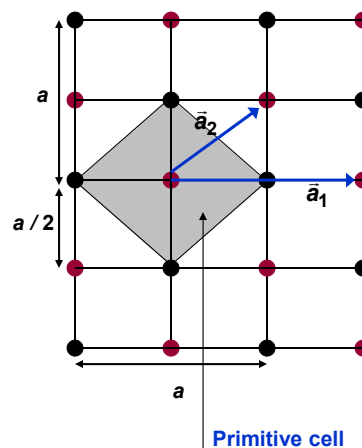
- The lattice primitive vectors are:

$$\vec{a}_1 = a \hat{x} \quad \vec{a}_2 = \frac{a}{2} \hat{x} + \frac{a}{2} \hat{y}$$

- The two basis vectors are:

$$\vec{d}_1 = 0$$

$$\vec{d}_2 = \frac{a}{2} \hat{x}$$

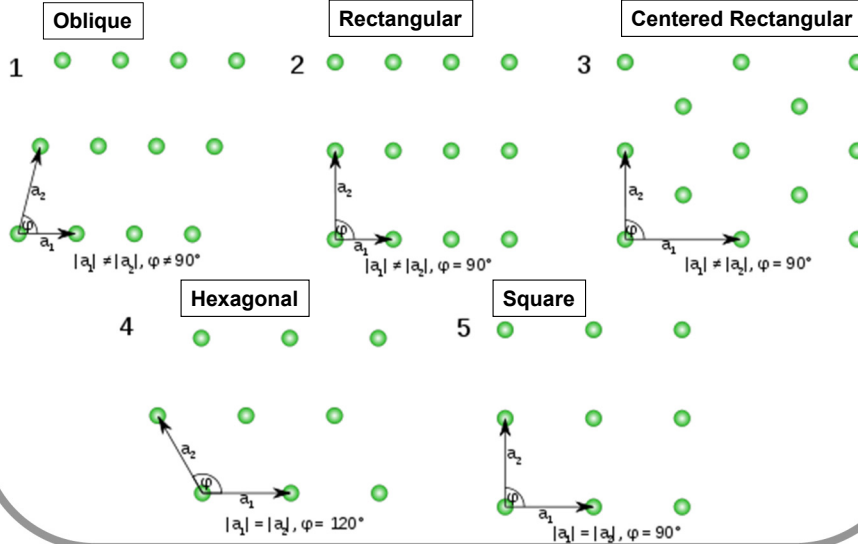


The primitive cell has the two basis atoms: one "red" and one "black" (actually one-fourth each of four "black" atoms)

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Bravais Lattices in 2D

There are only 5 Bravais lattices in 2D

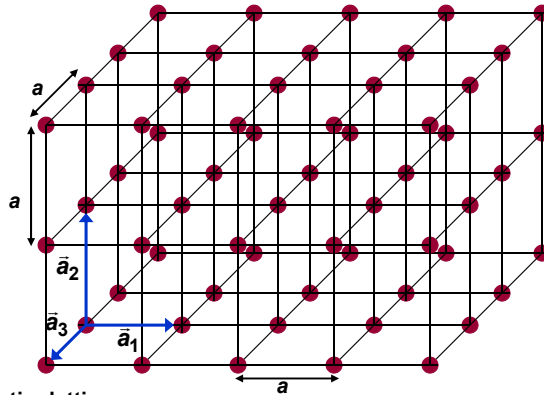
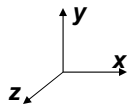


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Lattices in 3D and the Unit Cell

Simple Cubic Lattice:

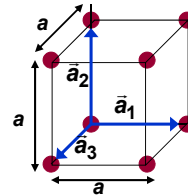
$$\begin{aligned} \bar{a}_1 &= a \hat{x} \\ \bar{a}_2 &= a \hat{y} \\ \bar{a}_3 &= a \hat{z} \end{aligned}$$



Unit Cell:

It is very cumbersome to draw entire lattices in 3D so some small portion of the lattice, having full symmetry of the lattice, is usually drawn. This small portion when repeated can generate the whole lattice and is called the “unit cell” and it could be larger than the primitive cell

Unit cell of a cubic lattice

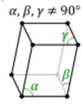


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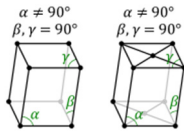
Bravais Lattices in 3D

There are 14 different Bravais lattices in 3D that are classified into 7 different crystal systems (only the **unit cells** are shown below)

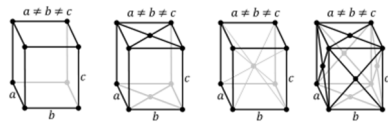
1) Triclinic:



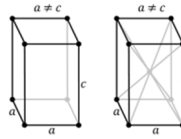
2) Monoclinic:



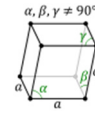
3) Orthorhombic:



4) Tetragonal:



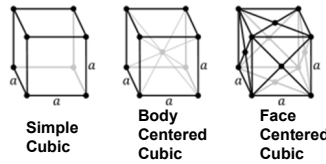
5) Rhombohedral:



6) Hexagonal:



7) Cubic:



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BCC and FCC Lattices

Body Centered Cubic (BCC) Lattice:

$$\bar{a}_1 = a \hat{x} \quad \bar{a}_2 = a \hat{y}$$

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

Or a more symmetric choice is:

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

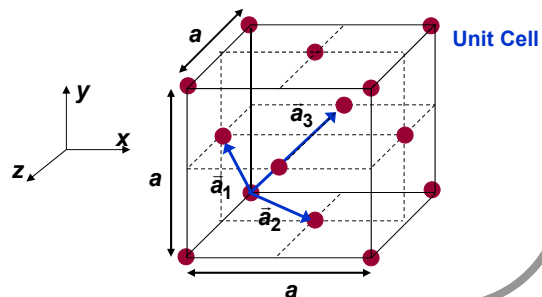
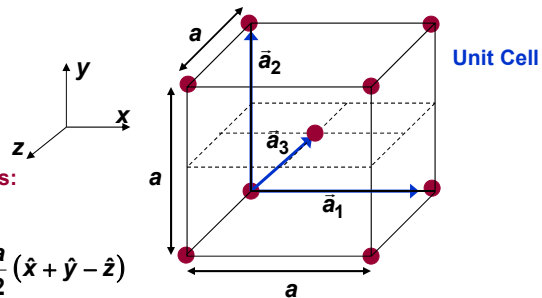
$$\bar{a}_2 = \frac{a}{2} (\hat{x} - \hat{y} + \hat{z}) \quad \bar{a}_3 = \frac{a}{2} (\hat{x} + \hat{y} - \hat{z})$$

Face Centered Cubic (FCC) Lattice:

$$\bar{a}_1 = \frac{a}{2} (\hat{y} + \hat{z})$$

$$\bar{a}_2 = \frac{a}{2} (\hat{x} + \hat{z})$$

$$\bar{a}_3 = \frac{a}{2} (\hat{x} + \hat{y})$$

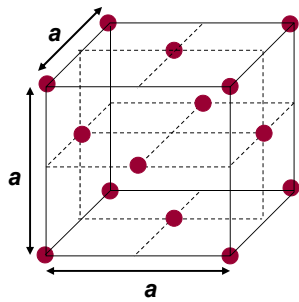


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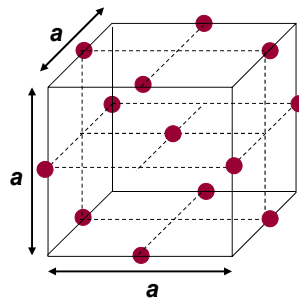
BCC and FCC Lattices

The choice of unit cell is not unique

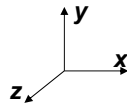
Shown are two different unit cells for the FCC lattice



FCC Unit Cell



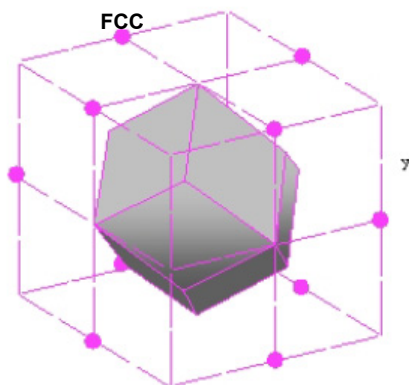
FCC Unit Cell



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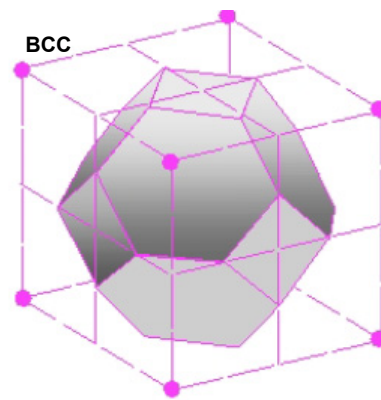
BCC and FCC Lattices

The (Wigner-Seitz) primitive cells of FCC and BCC Lattices are shown:



Materials with FCC lattices:

Aluminum, Nickel, Copper, Platinum,
Gold, Lead, Silver, Silicon,
Germanium, Diamond, Gallium
Arsenide, Indium Phosphide



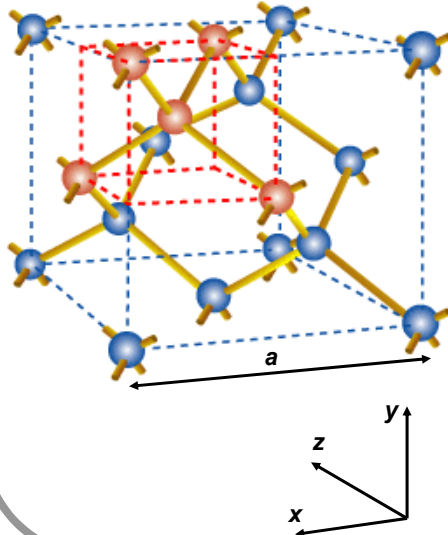
Materials with BCC lattices:

Lithium, Sodium, Potassium,
Chromium, Iron, Molybdenum,
Tungsten, Manganese

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Lattices of Silicon, Germanium, and Diamond

Diamond Lattice



- Each atom is covalently bonded to four other atoms via sp^3 bonds in a tetrahedral configuration
- The lattice defined by the position of the atoms is not a Bravais lattice
- The underlying lattice is an FCC lattice with a two-point (or two-atom) basis
- The lattice constant “ a ” usually found in the literature is the size of the unit cell, as shown. The **primitive lattice vectors** are:

$$\bar{a}_1 = \frac{a}{2}(\hat{y} + \hat{z}) \quad \bar{a}_2 = \frac{a}{2}(\hat{x} + \hat{z})$$

$$\bar{a}_3 = \frac{a}{2}(\hat{x} + \hat{y}) \quad \text{Same as for a FCC lattice}$$

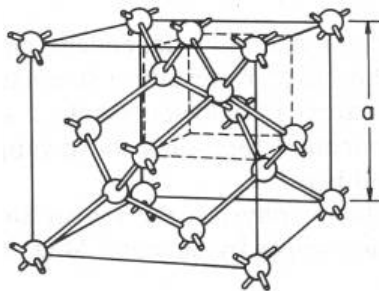
- The **two basis vectors** are:

$$\bar{d}_1 = 0 \quad \bar{d}_2 = \frac{a}{4}(\hat{x} + \hat{y} + \hat{z})$$

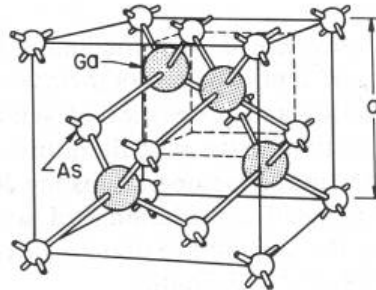
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Lattices of III-V Binaries (GaAs, InP, GaP, InAs, AlAs, InSb, etc)

Diamond lattice (Si, Ge, Diamond)



Zincblende lattice (GaAs, InP, InAs)



- Each Group III atom is covalently bonded to four other group V atoms (and vice versa) via sp^3 bonds in a tetrahedral configuration
- The underlying lattice is an FCC lattice with a two-point (or two-atom) basis. In contrast to the diamond lattice, the two atoms in the basis of zincblende lattice are different

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