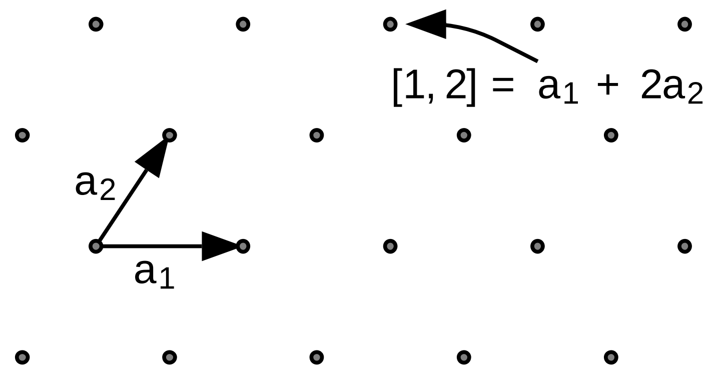
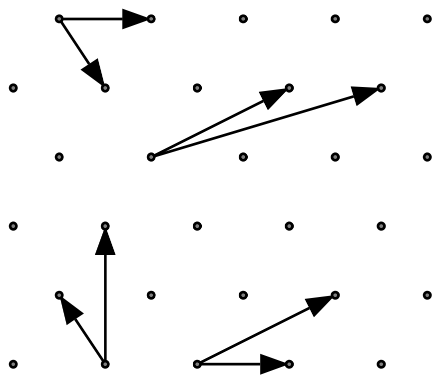
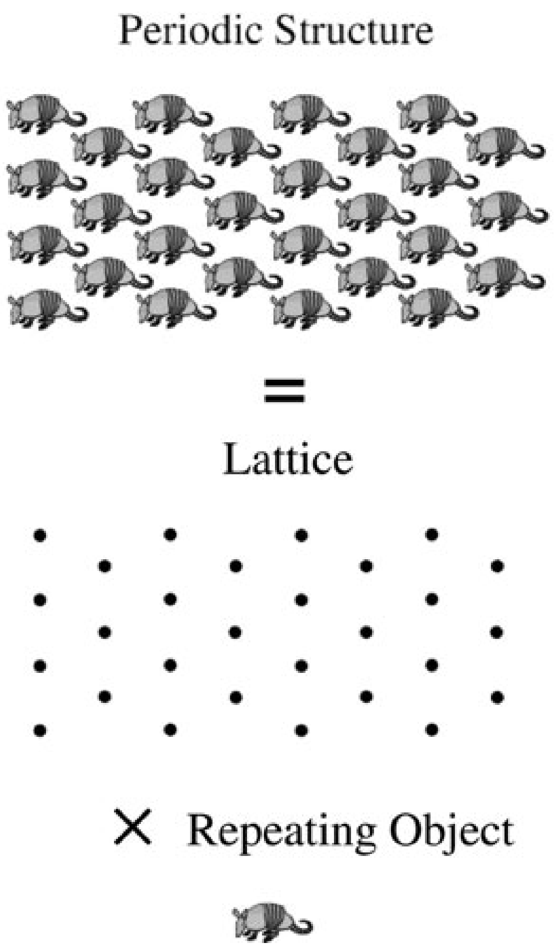
Crystal Structure

Lattices and Unit Cells







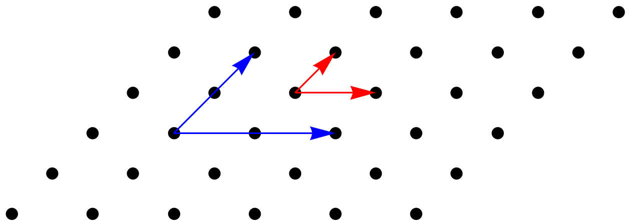
VESTA is an important tool for this class . Free to download and install

Primitive lattice vectors

For a 3D lattice, we can find three primitive lattice vectors (primitive translation vectors), such that any translation vector can be written as

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

where n_1, n_2 and n_3 are three integers.



Red (shorter) vectors: $\vec{a}_1$ and $\vec{a}_2$

Blue (longer) vectors: $\vec{b}_1$ and $\vec{b}_2$

$\vec{a}_1$ and $\vec{a}_2$ are primitive lattice vectors
$\vec{b}_1$ and $\vec{b}_2$ are NOT primitive lattice vectors

$$\vec{b}_1 = 2\vec{a}_1 + 0\,\vec{a}_2$$

Integer coefficients

$$\vec{a}_1 = \frac{1}{2}\vec{b}_1 + 0\vec{b}_2$$

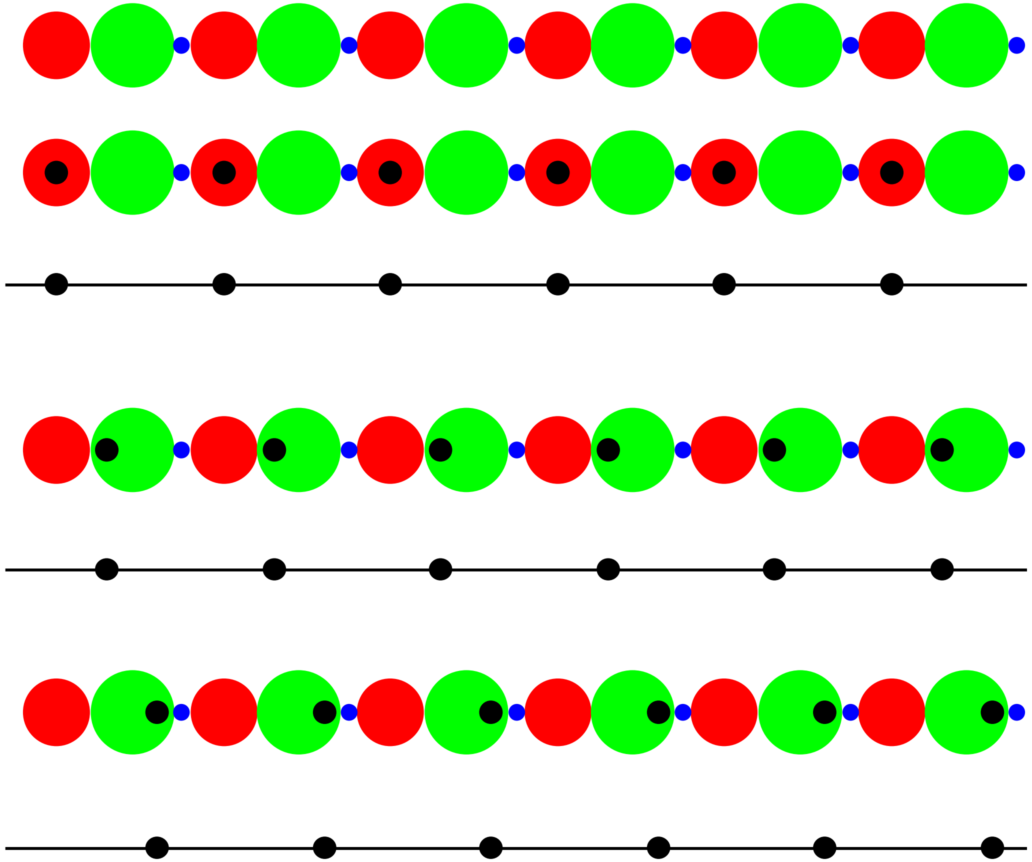
noninteger coefficients

1D crystal
3 atoms/periodicity

Choice I:

Choice II:

Choice III:

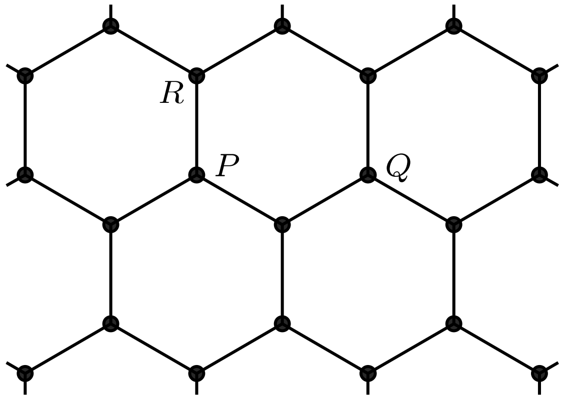


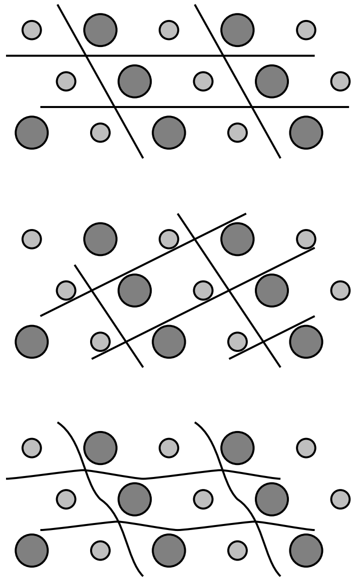
1D crystal
3 atoms/periodicity

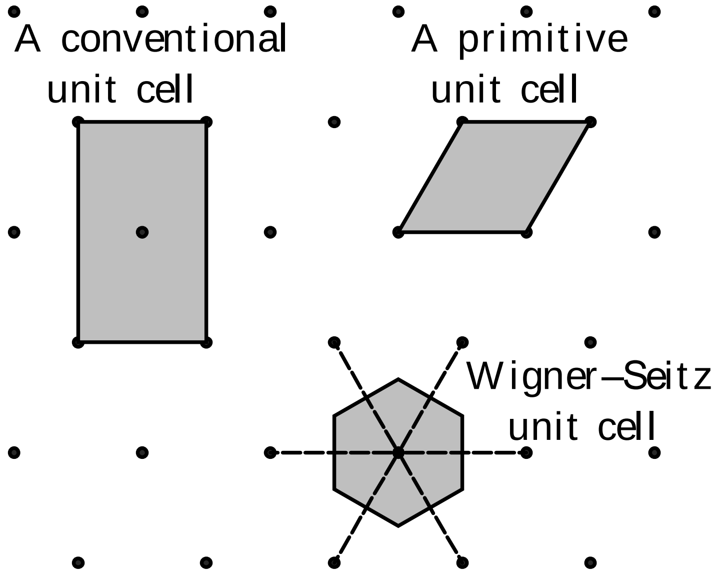
Choice I:

Choice II:

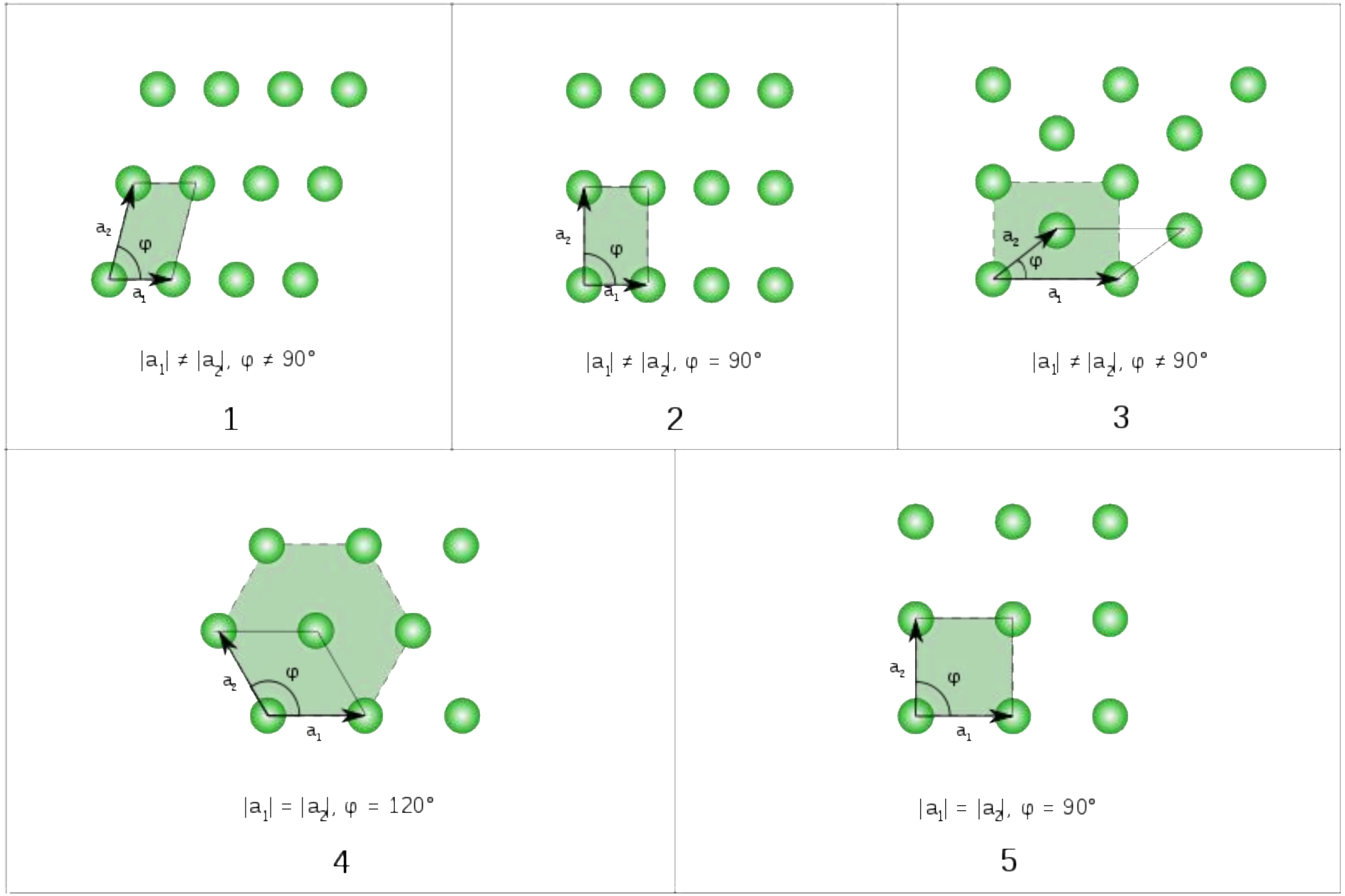
Choice III:


R
P
Q



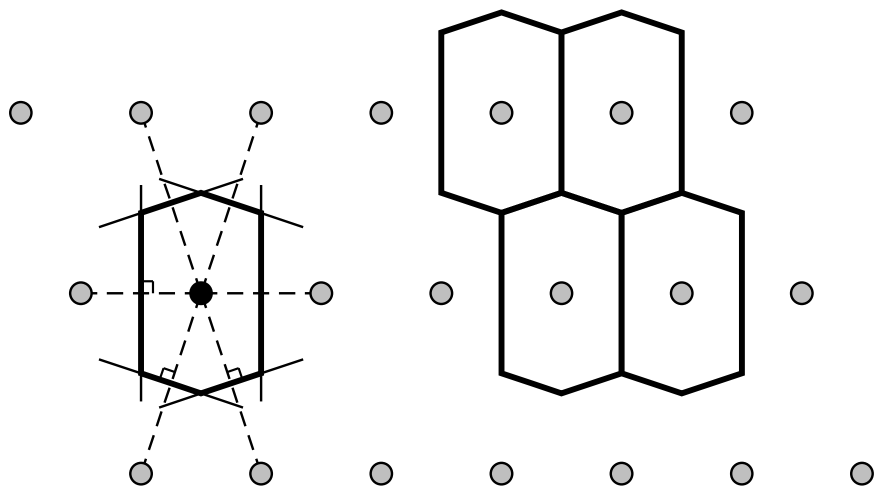

A conventional unit cell
A primitive unit cell
Wigner–Seitz unit cell

5 Bravaus lattices in 2D

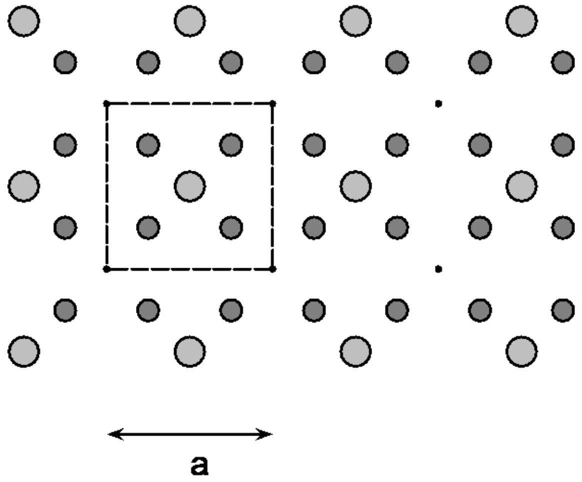


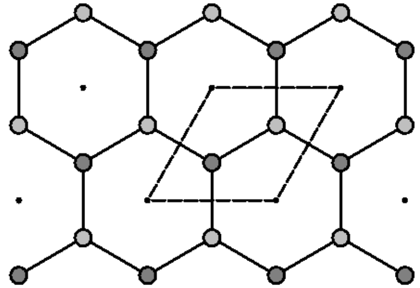
http://en.wikipedia.org/wiki/Bravais_lattice

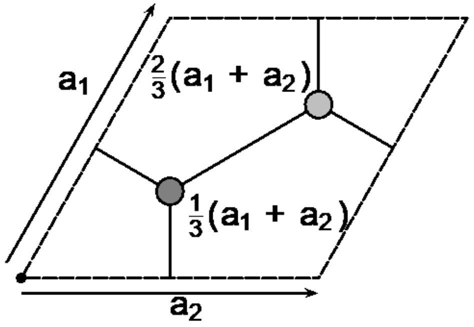
Wigner Seitz construction

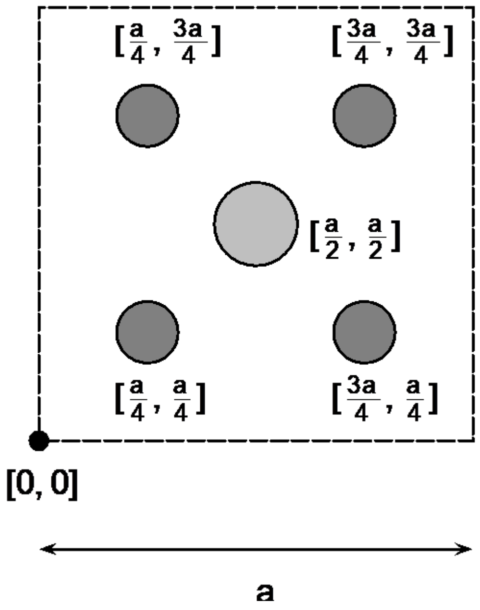


Basis and location of atoms in unit cell









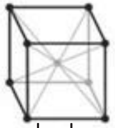
To remember: CRYSTAL = LATTICE + BASIS

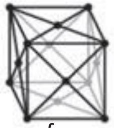
Lattices in Three Dimensions

14 Bravaus lattices in 3D

cubic:


simple

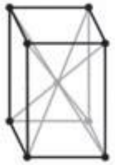

body centered


face centered

cubic:
all sides equal
all angles 90°

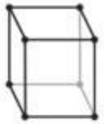
tetragonal:


simple


body centered

tetragonal:
only two of three side lengths equal
all angles 90°

orthorhombic:


simple

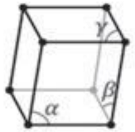

body centered


face centered


base centered

orthorhombic:
no two sides equal
all angles 90°

simple monoclinic

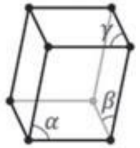


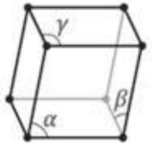
base centered monoclinic

monoclinic:
angles between primitive lattice vectors :
$\alpha = 90°$ $\beta = 90°$
$\alpha \neq 90°$
only two right angles

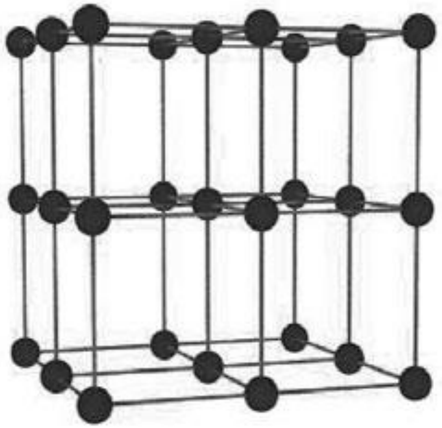
hexagonal

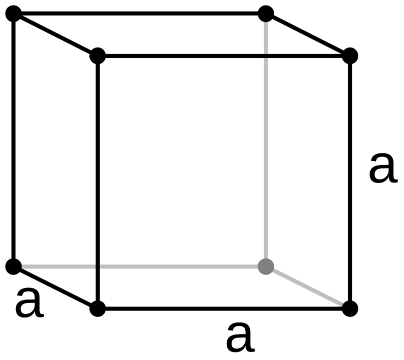
triclinic:
no right angles
no two sides equal



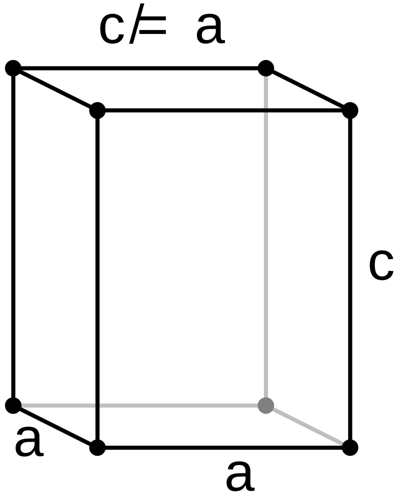


rhombohedral:
all side lengths equal.
all angles equal, but not right angles.

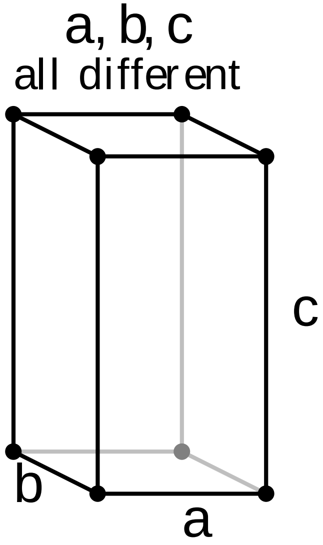




Cubic
unit cell

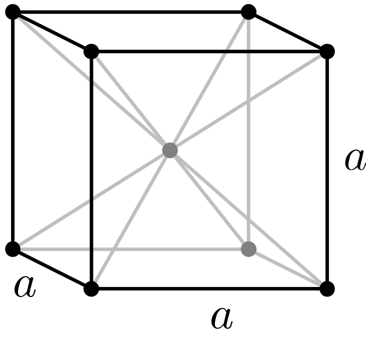


Tetragonal
unit cell

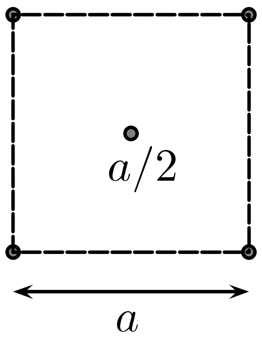


Orthorhombic
unit cell

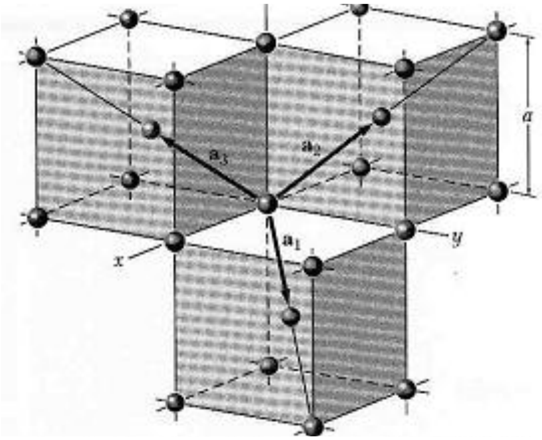
The Body-Centered Cubic (bcc) Lattice

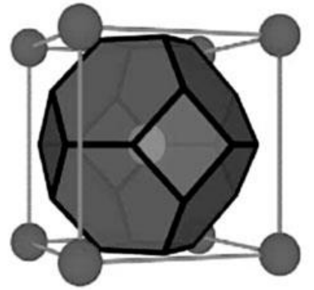


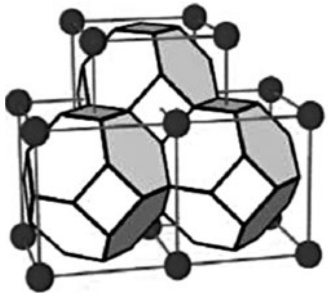
Body-centered cubic
unit cell



Plan view







Lattice sites: $a(l\,\hat{x} + m\,\hat{y} + n\,\hat{z})$

Lattice point per conventional cell: $1 = 8 \times \frac{1}{8}$

Volume (conventional cell): a^3

Volume (primitive cell): a^3

Number of nearest neighbors: 6

Nearest neighbor distance: a

Number of second neighbors: 12

Second neighbor distance: $\sqrt{2}a$

Coordinates of the sites: (l, n, m)

For the site $(0,0,0)$,

6 nearest neighbors: $(\pm1,0,0)$, $(0,\pm1,0)$ and $(0,0,\pm1)$

12 nest nearest neighbors: $(\pm1,\pm1,0)$, $(0,\pm1,\pm1)$ and $(\pm1,0,\pm1)$

Packing fraction

Packing fraction:

We try to pack N spheres (hard, cannot deform).

The total volume of the spheres is $N 4\pi \frac{R^3}{3}$

The volume these spheres occupy $V > N 4\pi \frac{R^3}{3}$ (there are spacing)

Packing fraction=total volume of the spheres/total volume these spheres occupy

$$Packing\ fraction = \frac{N 4\pi \frac{R^3}{3}}{V} = \frac{4\pi \frac{R^3}{3}}{V/N} = \frac{4\pi \frac{R^3}{3}}{Volume\ per\ site}$$

$$= \frac{4\pi \frac{R^3}{3}}{Volume\ of\ a\ primitive\ cell}$$

High packing fraction means the space is used more efficiently

Packing fraction of simple cubic

$$Packing\ fraction = \frac{4\pi \frac{R^3}{3}}{Volume\ of\ a\ primitive\ cell}$$

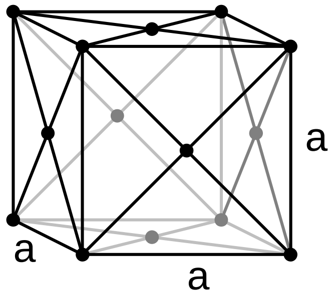
$$= \frac{4\pi \frac{R^3}{3}}{a^3} = \frac{4\pi}{3}\left(\frac{R}{a}\right)^3 = \frac{4\pi}{3}\left(\frac{a/2}{a}\right)^3 = \frac{\pi}{6} \approx 0.524$$

Nearest distance = 2R

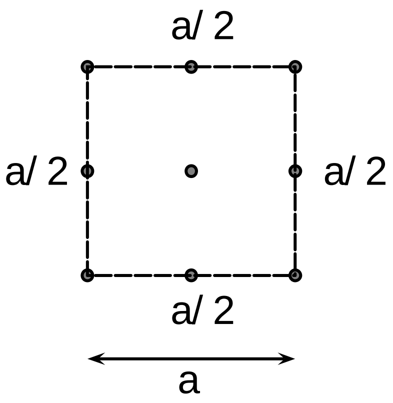
R = Nearest distance/2 = $a/2$

- About half (0.524=52.4%) of the space is really used by the sphere.
- The other half (0.476=47.6%) is empty.

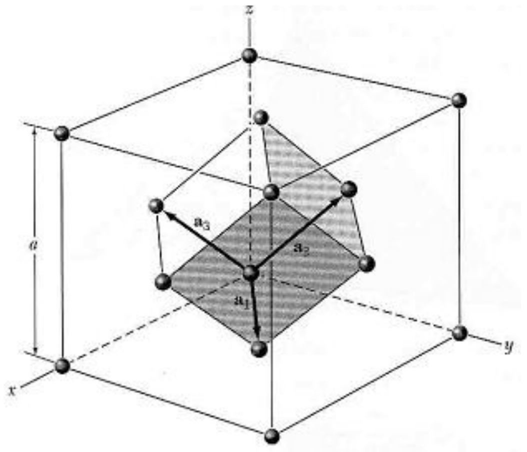
The Face-Centered Cubic (fcc) Lattice

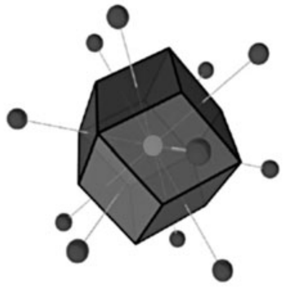


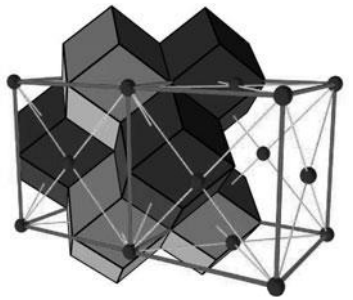
Face-centered cubic
unit cell



Plan view





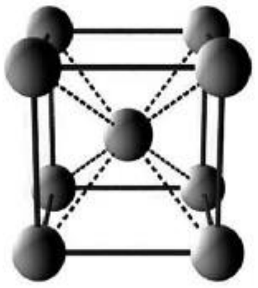


Some Real Crystals

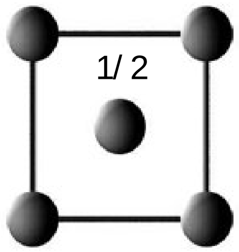
Sodium (Na)

Lattice = Cubic-I (bcc)

Basis = Na at [000]



Plan view
unlabeled points at z = 0, 1

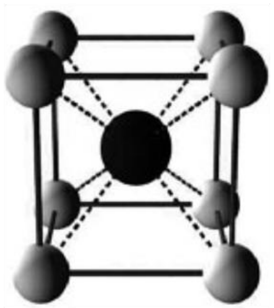


Caesium chloride (CsCl)

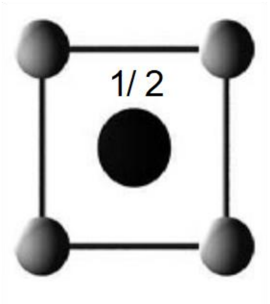
Lattice = Cubic-P

Basis = Cs at [000]

and Cl at $[\frac{1}{2}\frac{1}{2}\frac{1}{2}]$



Plan view
unlabeled points at z = 0, 1



We can mark any unit cell by three integers: lmn

$$\vec{t} = l\vec{a}_1 + m\,\vec{a}_2 + n\,\vec{a}_3$$

Coordinates of an atom:

We can mark any atom in a unit cell by three real numbers: xyz.

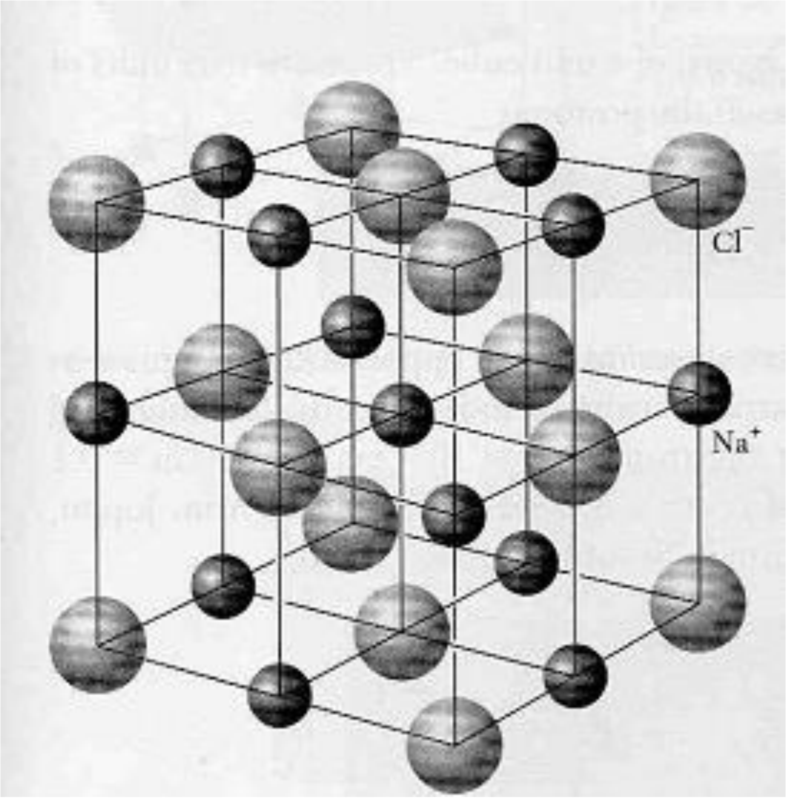
The location of this atom: $x\,\vec{a}_1 + y\,\vec{a}_2 + z\,\vec{a}_3$

Notice that $0 \le x < 1$ and $0 \le y < 1$ and $0 \le z < 1$

Q: Why x cannot be 1?

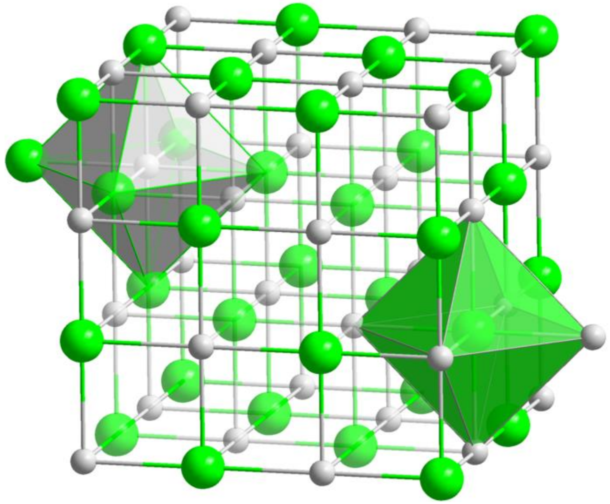
A: Due to the periodic structure. 1 is just 0 in the next unit cell

Sodium Chloride



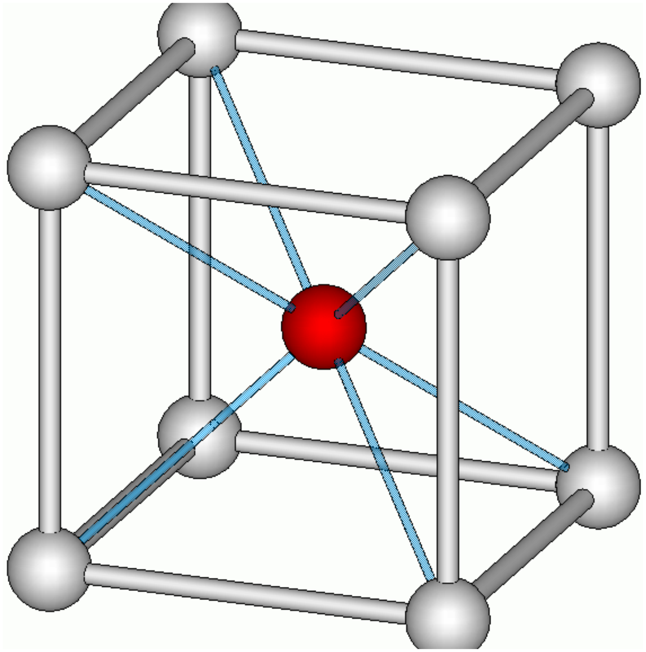
Face-centered cubic lattice
Na+ ions form a face-centered cubic lattice
Cl- ions are located between each two neighboring Na+ ions

Equivalently, we can say that
Cl- ions form a face-centered cubic lattice
Na+ ions are located between each two neighboring Na+ ions



Primitive cells

Cesium Chloride



Simple cubic lattice
Cs+ ions form a cubic lattice
Cl- ions are located at the center of each cube

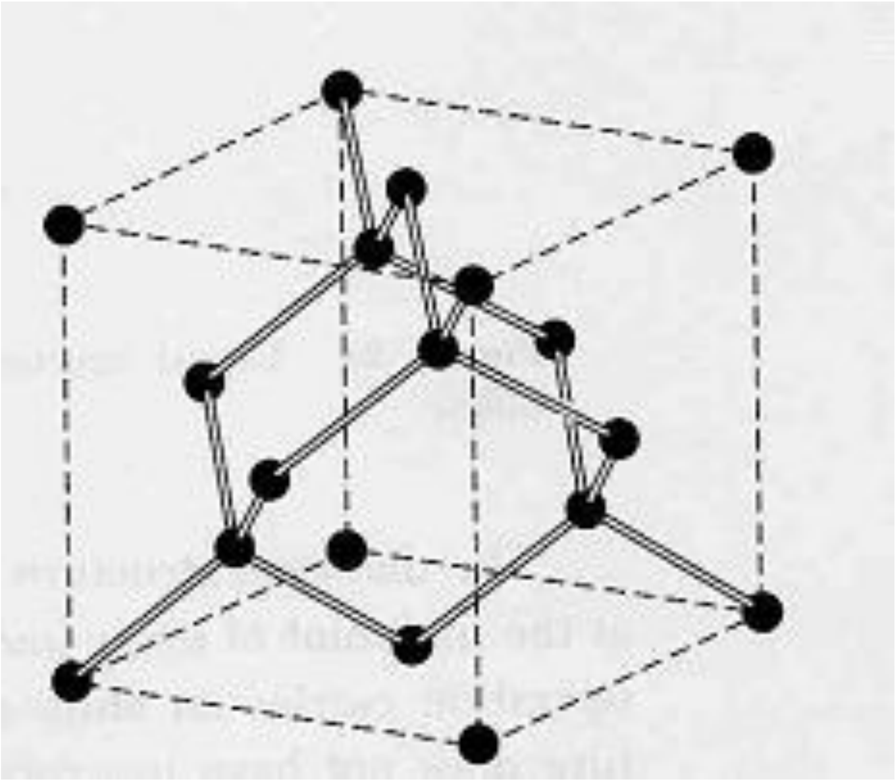
Equivalently, we can say that
Cl- ions form a cubic lattice
Cs+ ions are located at the center of each cube

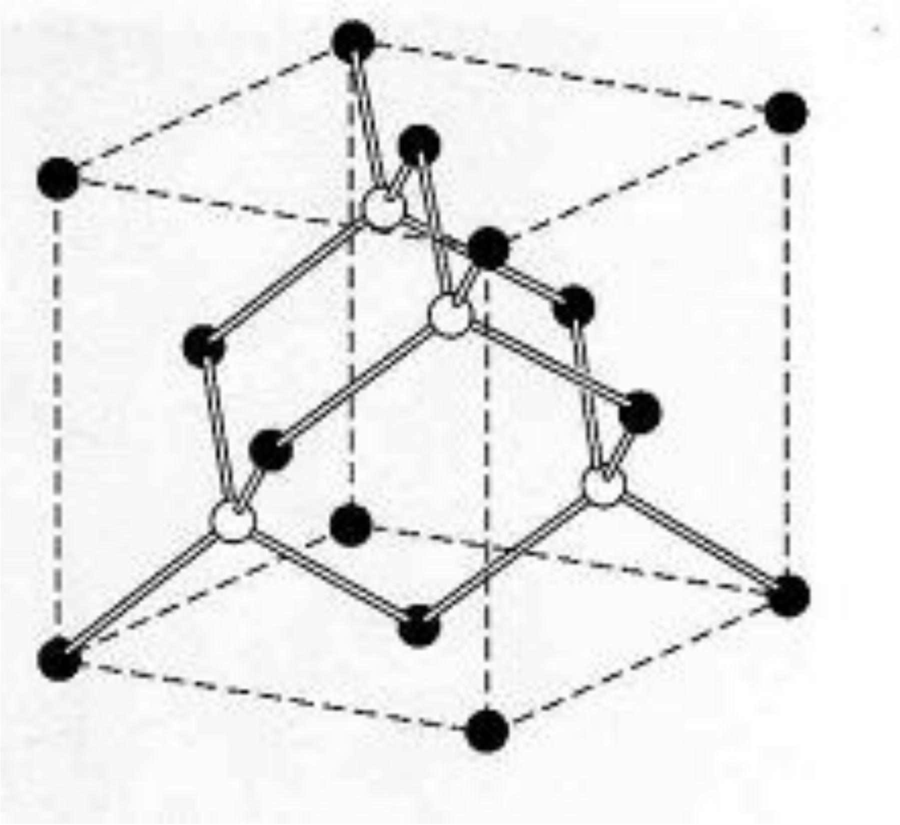
Coordinates:
Cs: 000
Cl: $\frac{1}{2}\frac{1}{2}\frac{1}{2}$

Notice that this is a simple cubic lattice
NOT a body centered cubic lattice

- For a bcc lattice, the center site is the same as the corner sites
- Here, center sites and corner sites are different

Diamond is not a Bravais lattice

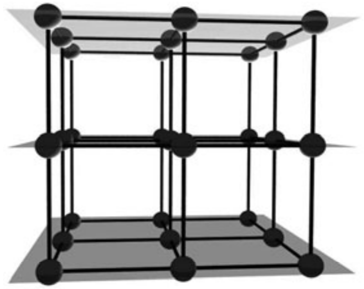




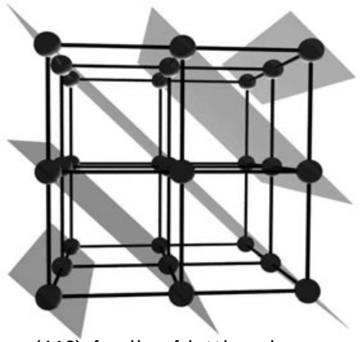
Same story as in graphene:
We can distinguish two different type of carbon sites (marked by different color)
We need to combine two carbon sites (one black and one white) together as a (primitive) unit cell
If we only look at the black (or white) sites, we found the Bravais lattice: fcc

Reciprocal lattice and Brillouin Zone

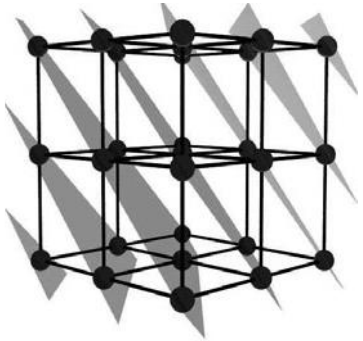
Examples of families of lattice planes on the cubic lattice. Each of these planes is a lattice plane because it intersects at least three non-collinear lattice points.



(010) family of lattice planes



(110) family of lattice planes



(111) family of lattice planes