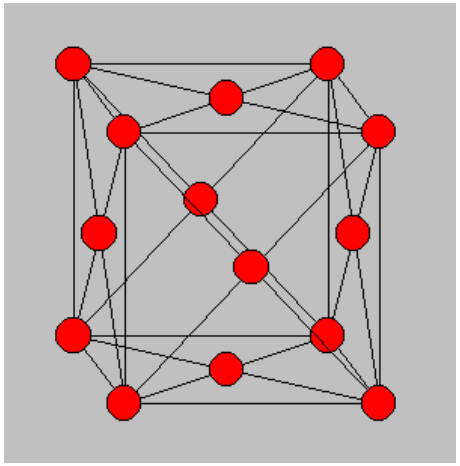
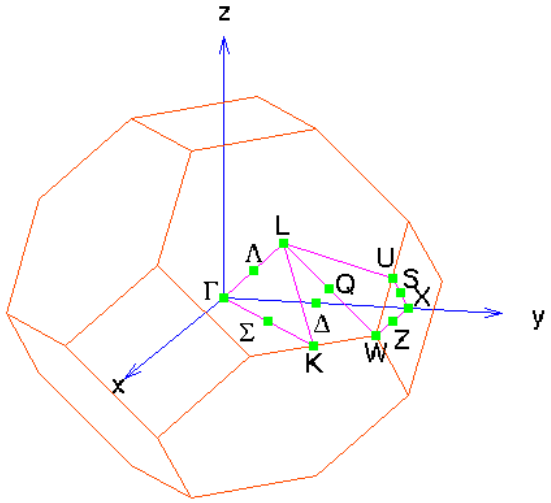
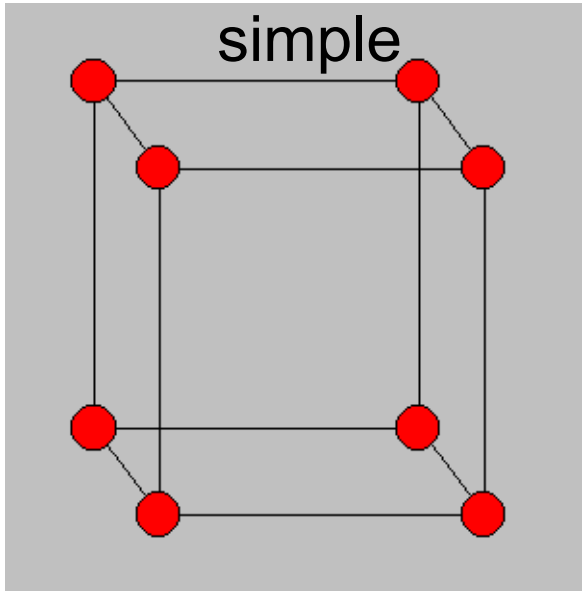
PH575 Spring 2019

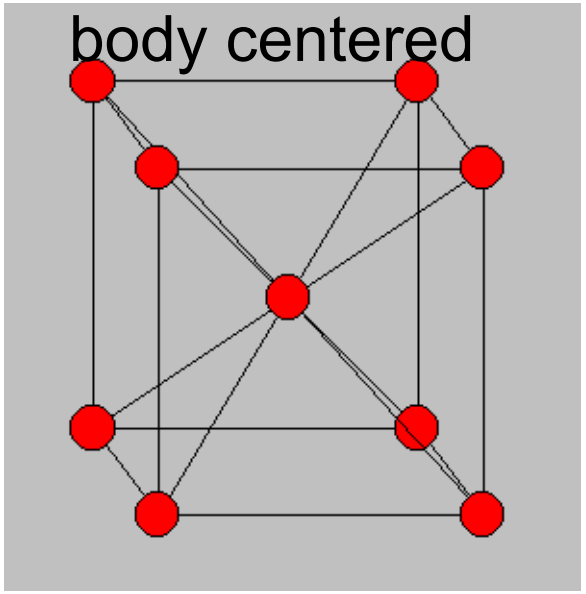
Lecture #12
3 dimensions: Sutton Ch. 4 pp 78-> 80; Kittel Ch1, 2

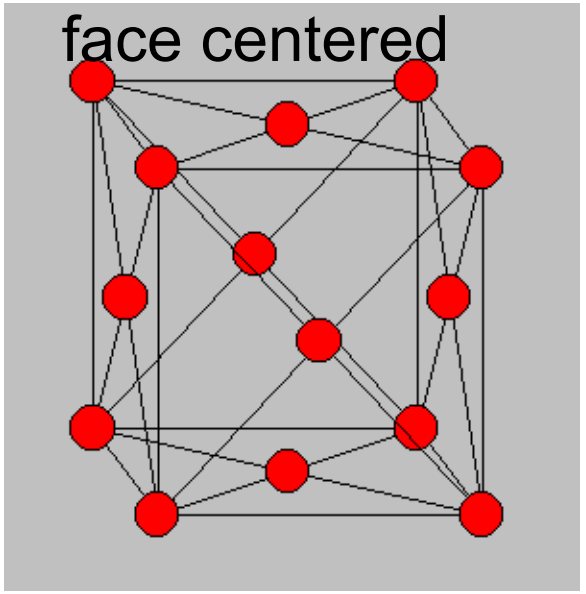


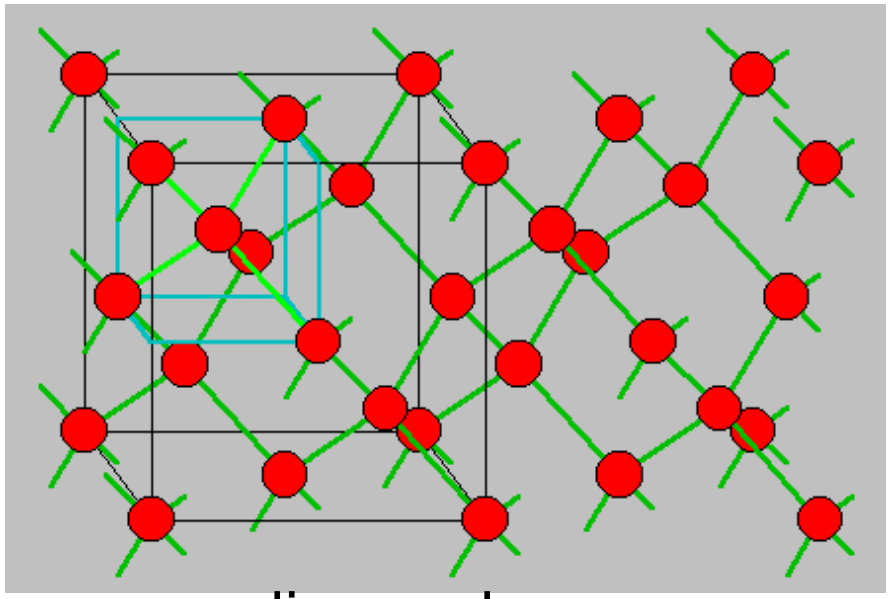


The cubic lattices

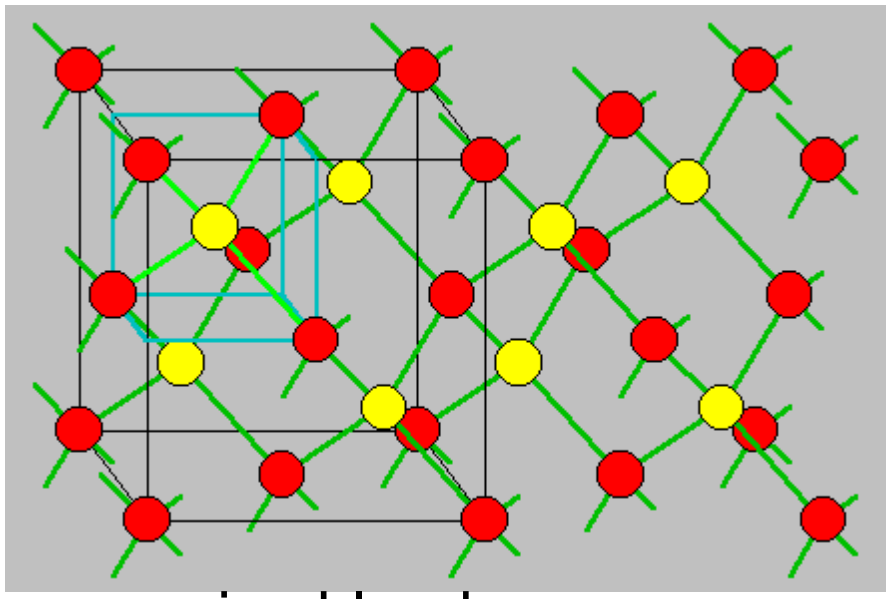






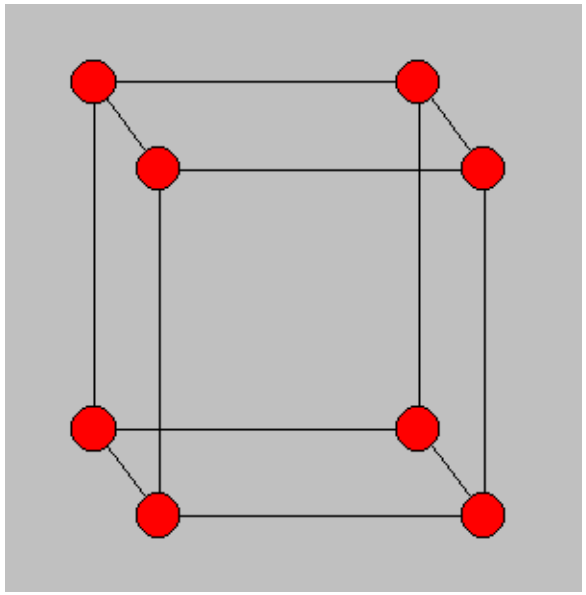


diamond



zinc blende

Simple cubic lattice
in real space (or direct lattice)



- Unit cell generates entire lattice by repetition and covers all space.
- Every atom can be reached by
- $\mathbf{R} = n\,\mathbf{t}_1 + m\,\mathbf{t}_2 + p\mathbf{t}_3$
- Primitive cell is a unit cell that contains one fundamental unit (in this case 1 atom) or lattice cell.
- Volume is

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

$\mathbf{t}_1 = (\,a\,,\,0\,,\,0\,)$
$\mathbf{t}_2 = (\,0\,,\,a\,,\,0\,)$
$\mathbf{t}_3 = (\,0\,,\,0\,,\,a\,)$

Construct **reciprocal lattice**

The real space (direct) lattice vectors are $\vec{t}_1, \vec{t}_2, \vec{t}_3$

then the reciprocal lattice vectors are $\vec{g}_1, \vec{g}_2, \vec{g}_3$

$$\vec{g}_1 = 2\pi \frac{\vec{t}_2 \times \vec{t}_3}{\vec{t}_1 \cdot \left(\vec{t}_2 \times \vec{t}_3\right)}$$

$$\vec{g}_2 = 2\pi \frac{\vec{t}_3 \times \vec{t}_1}{\vec{t}_2 \cdot \left(\vec{t}_3 \times \vec{t}_1\right)}$$

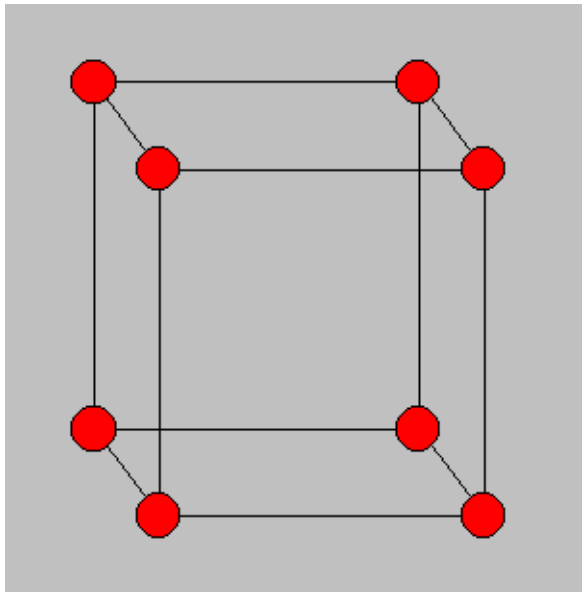
$$\vec{g}_3 = 2\pi \frac{\vec{t}_1 \times \vec{t}_2}{\vec{t}_3 \cdot \left(\vec{t}_1 \times \vec{t}_2\right)}$$

Also easy to see that

$$\vec{t}_i \cdot \vec{g}_j = 2\pi\delta_{ij}$$

$$e^{i\vec{g}\cdot\vec{t}} = 1$$

Simple cubic lattice in real space

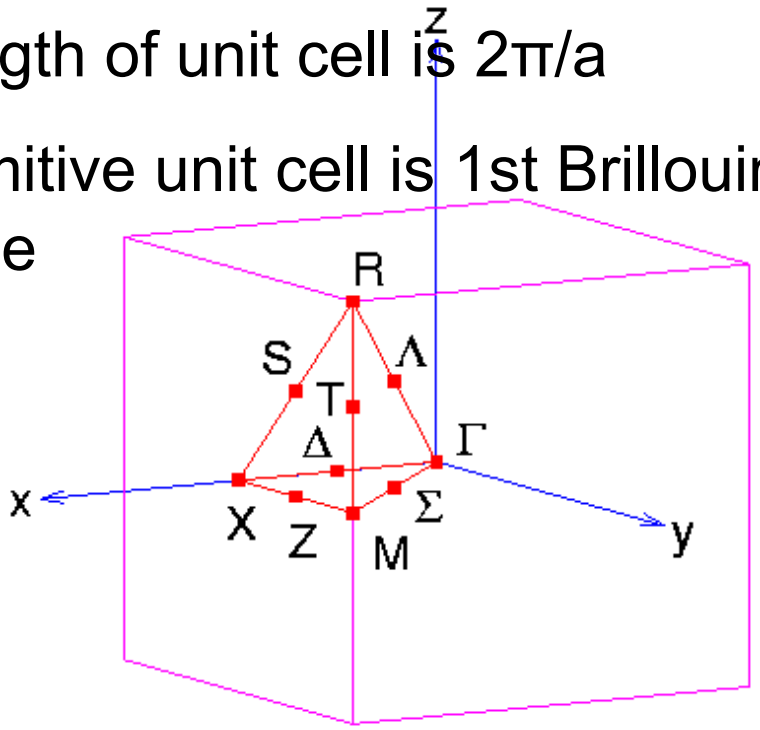


$\mathbf{t}_1 = (a , 0 , 0)$
$\mathbf{t}_2 = (0 , a , 0)$
$\mathbf{t}_3 = (0 , 0 , a)$

Reciprocal lattice is also simple cubic.

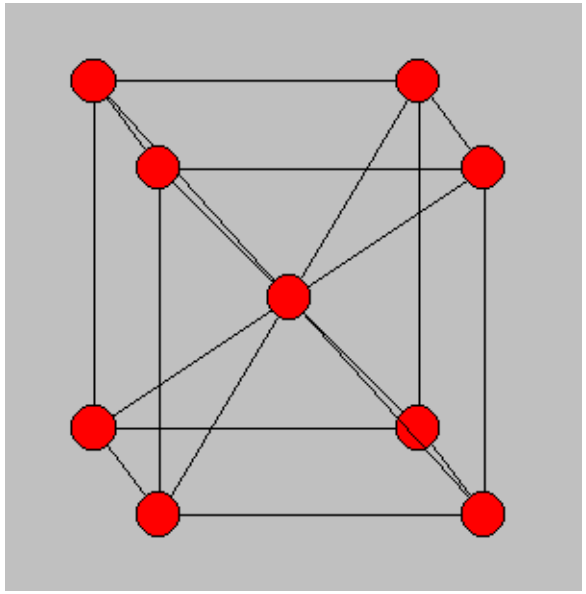
Length of unit cell is $2\pi/a$

Primitive unit cell is 1st Brillouin Zone

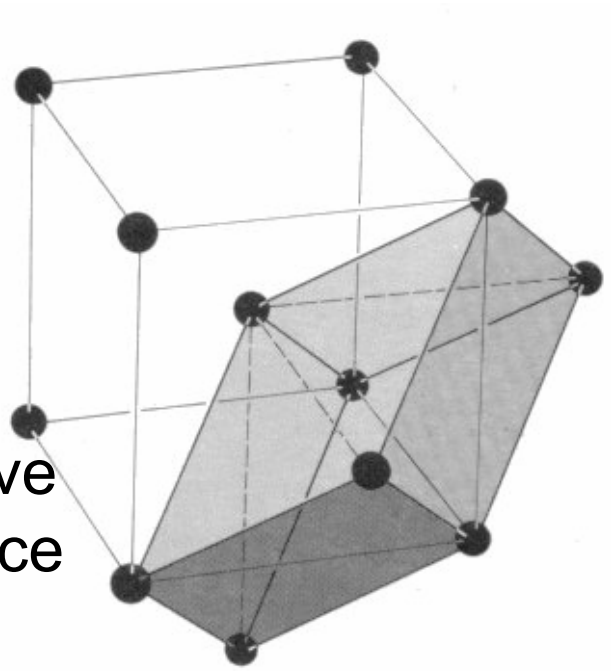


$\mathbf{g}_1 = (2\pi/a , 0 , 0)$
$\mathbf{g}_2 = (0 , 2\pi/a , 0)$
$\mathbf{g}_3 = (0 , 0 , 2\pi/a)$

http://cst-www.nrl.navy.mil/bind/kpts/sc/



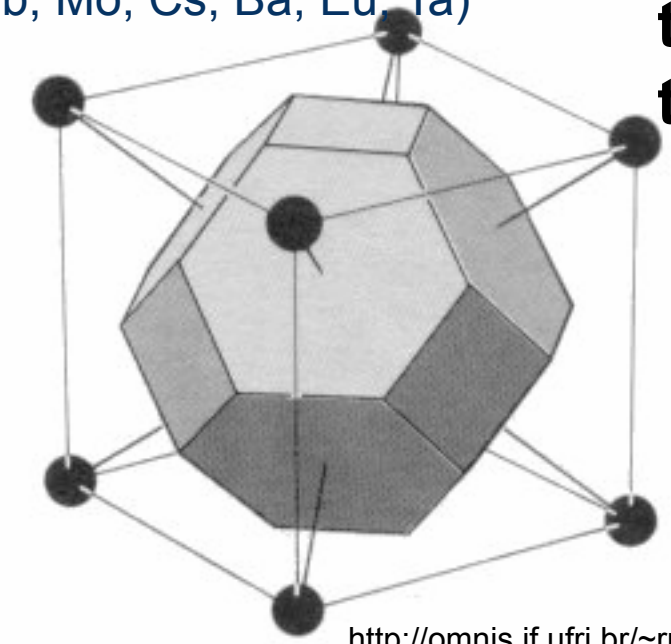
Conventional unit cell
Has full lattice symmetry
2 atoms/cell



Primitive unit cell
Does not always have
full symmetry of lattice
1 atoms/cell

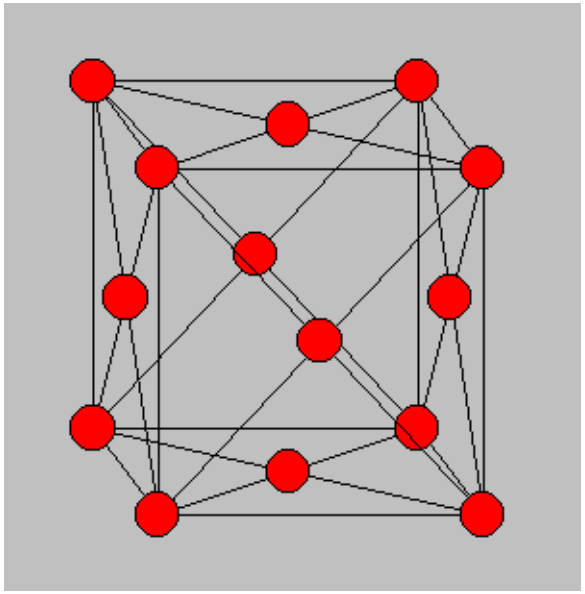
Body centered cubic lattice
(Li(@RT), Na, K, V, Cr, Fe, Rb, Nb, Mo, Cs, Ba, Eu, Ta)

$\mathbf{t}_1 = (a/2)\ (-1,\ 1\ ,\ 1)$
$\mathbf{t}_2 = (a/2)\ (1\ ,\ -1\ ,\ 1)$
$\mathbf{t}_3 = (a/2)\ (1\ ,\ 1,\ -1)$

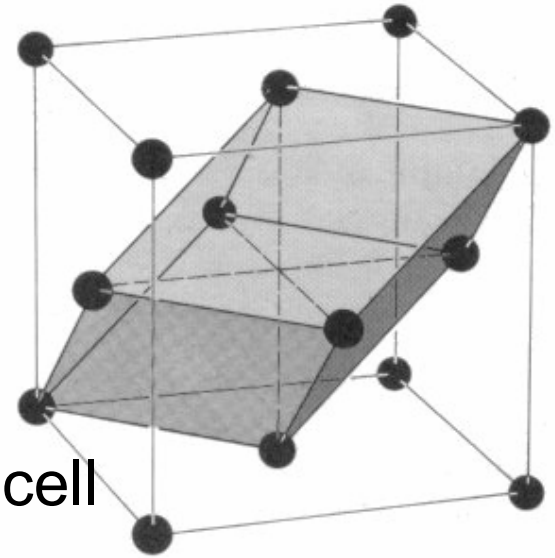


Another primitive cell:
Wigner-Seitz unit cell
1 atoms/cell & all points
as compact as possible
(b.t.w = 1st BZ of fcc!)

http://omnis.if.ufrj.br/~rrds/cursos/matcond/cap04/redes-3d.h



Conventional unit cell
4 atoms/cell



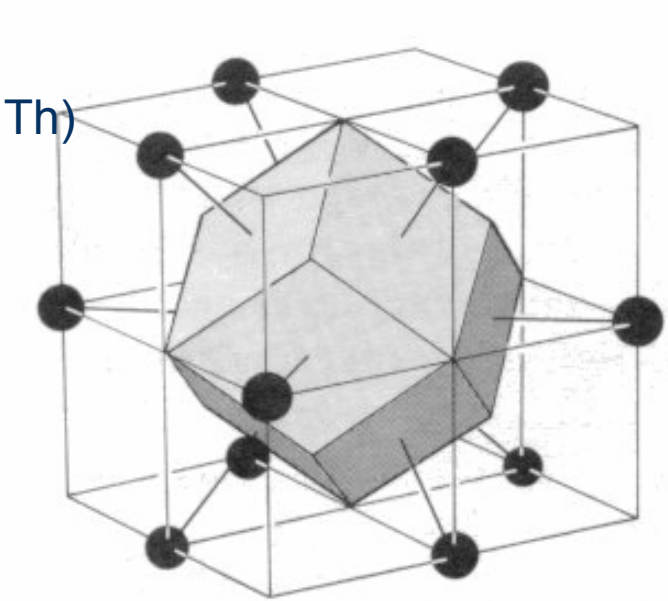
Primitive cell

$\mathbf{t}_1 = (a/2)\ (0, 1, 1)$
$\mathbf{t}_2 = (a/2)\ (1, 0, 1)$
$\mathbf{t}_3 = (a/2)\ (1, 1, 0)$

Face centered cubic lattice

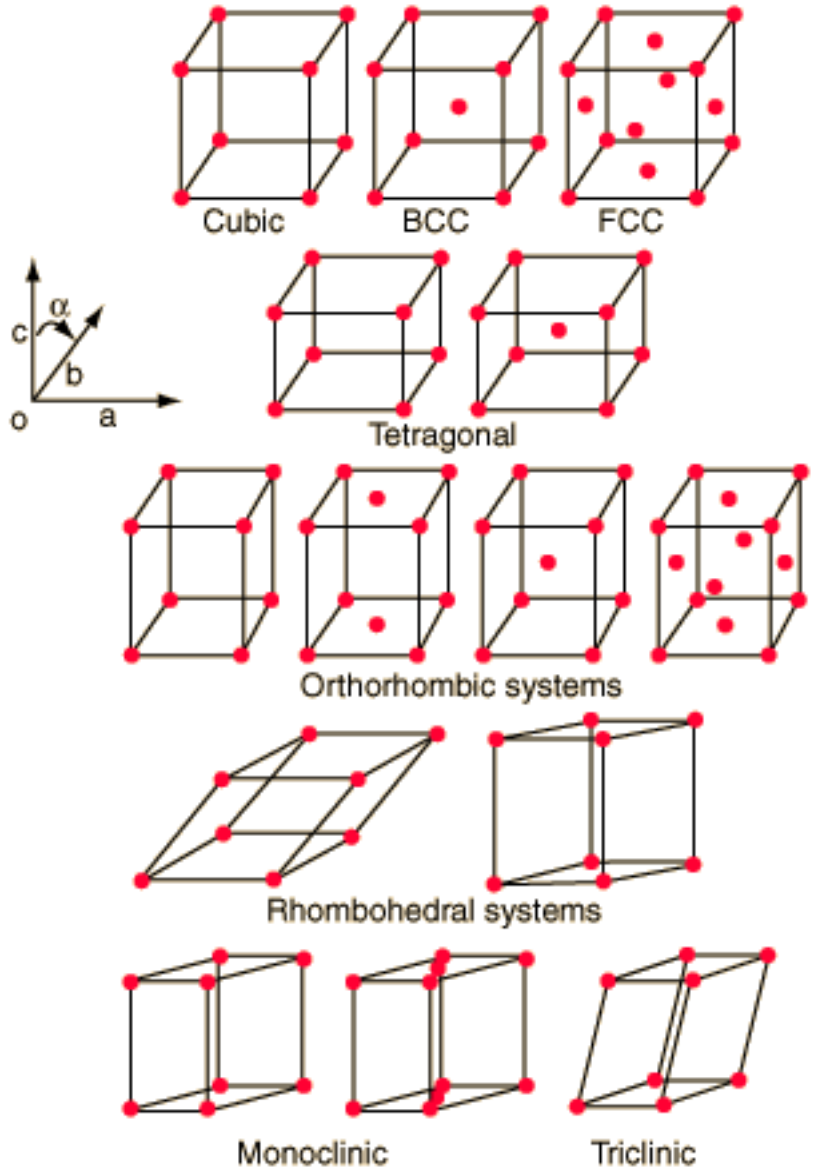
(Al, Cu, Ni, Sr, Rh, Pd, Ag, Ce, Tb, Ir, Pt, Au, Pb, Th)

Wigner-Seitz unit cell
(b.t.w = 1st BZ of bcc!)



http://omnis.if.ufrj.br/~rrds/cursos/matcond/cap04/redes-3d.h

The 14 Bravais Lattices



Auguste Bravais (1811-1863)

The reciprocal lattice vectors of the BCC lattice

The real lattice vectors of the BCC lattice

$\mathbf{t}_1 = (a/2)\,(-1,\ 1\ ,\ 1)$
$\mathbf{t}_2 = (a/2)\,(1\ ,\ -1\ ,\ 1)$
$\mathbf{t}_3 = (a/2)\,(1\ ,\ 1,\ -1)$

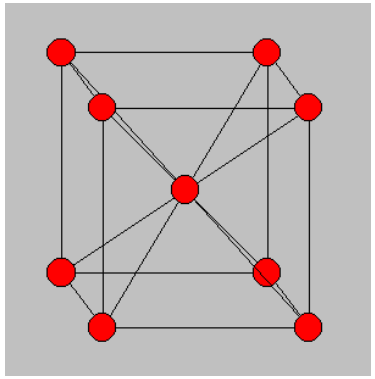
$$\vec{g}_1 = 2\pi \frac{\left(2\hat{y} + 2\hat{z}\right)}{\frac{a}{2}\left(-\hat{x} + \hat{y} + \hat{z}\right)\cdot\left(2\hat{y} + 2\hat{z}\right)} = \frac{2\pi}{a}\left(\hat{y} + \hat{z}\right)$$

$$\vec{g}_2 = 2\pi \frac{\left(2\hat{x} + 2\hat{z}\right)}{\frac{a}{2}\left(\hat{x} - \hat{y} + \hat{z}\right)\cdot\left(2\hat{x} + 2\hat{z}\right)} = \frac{2\pi}{a}\left(\hat{x} + \hat{z}\right)$$

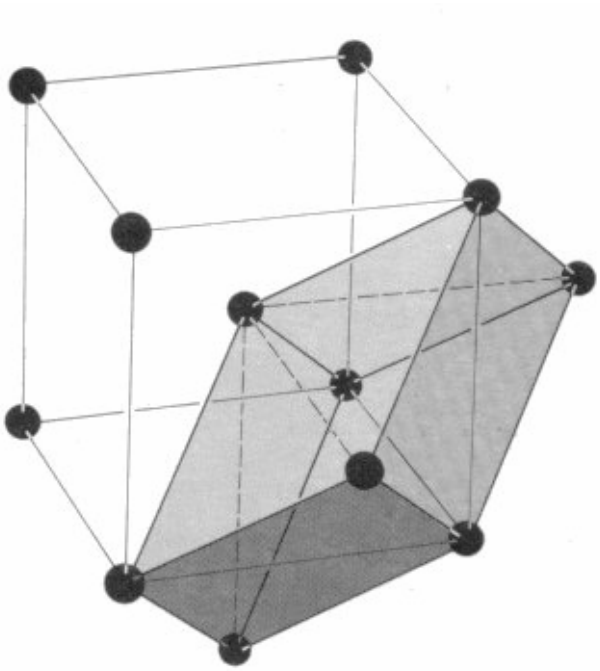
$$\vec{g}_3 = 2\pi \frac{\left(2\hat{x} + 2\hat{y}\right)}{\frac{a}{2}\left(\hat{x} + \hat{y} - \hat{z}\right)\cdot\left(2\hat{x} + 2\hat{y}\right)} = \frac{2\pi}{a}\left(\hat{x} + \hat{y}\right)$$

The reciprocal lattice vectors of the BCC lattice are also the real space vectors of the FCC lattice!

$\mathbf{g}_1 = (2\pi/a)(\ 0\ ,\ 1\ ,\ 1)$
$\mathbf{g}_2 = (2\pi/a)\ (1\ ,\ 0\ ,\ 1)$
$\mathbf{g}_3 = (2\pi/a)\ (1,\ 1,\ 0)$

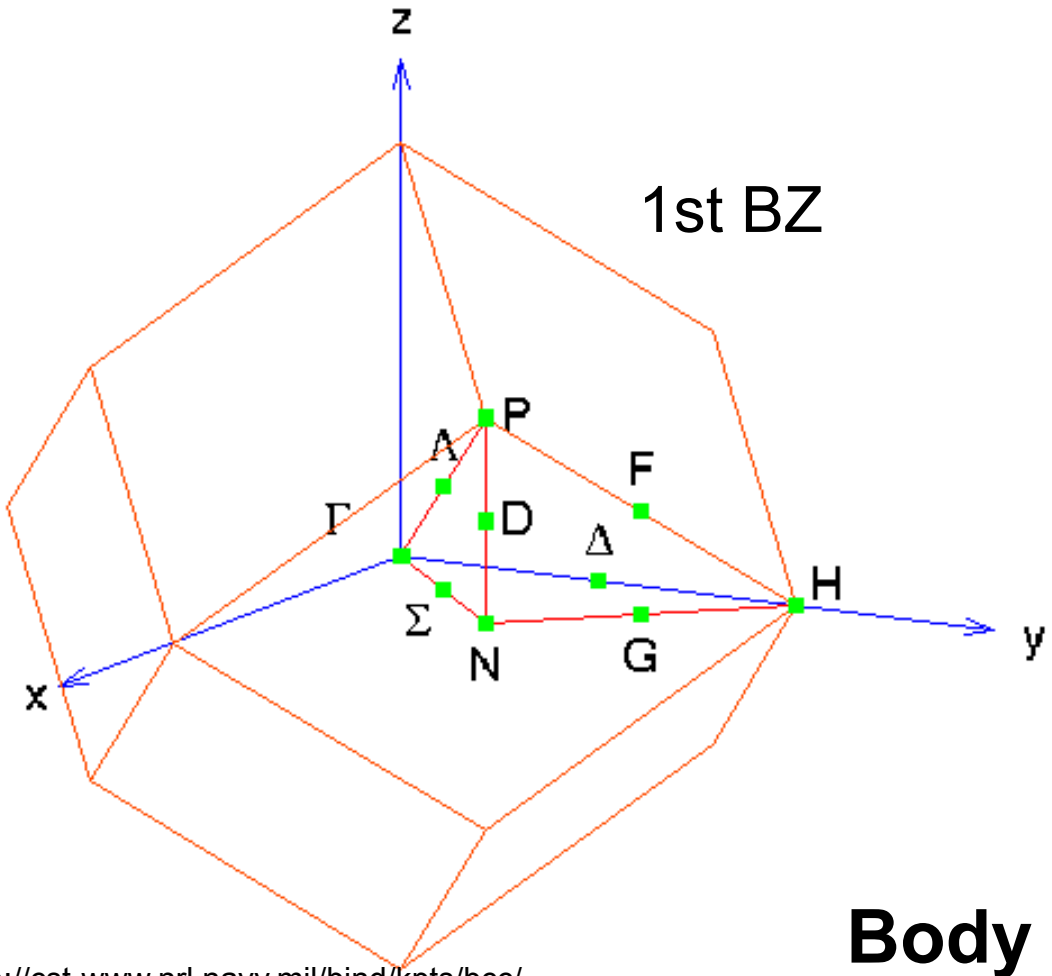


Primitive unit cell
Does not always have full symmetry of lattice
1 atoms/cell



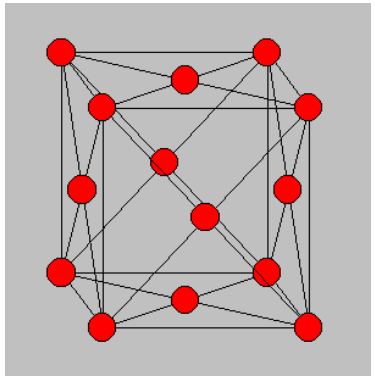
$\mathbf{t}_1 = (a/2)\ (-1,\ 1\ ,\ 1)$
$\mathbf{t}_2 = (a/2)\ (1\ ,\ -1\ ,\ 1)$
$\mathbf{t}_3 = (a/2)\ (1\ ,\ 1,\ -1)$

1st BZ

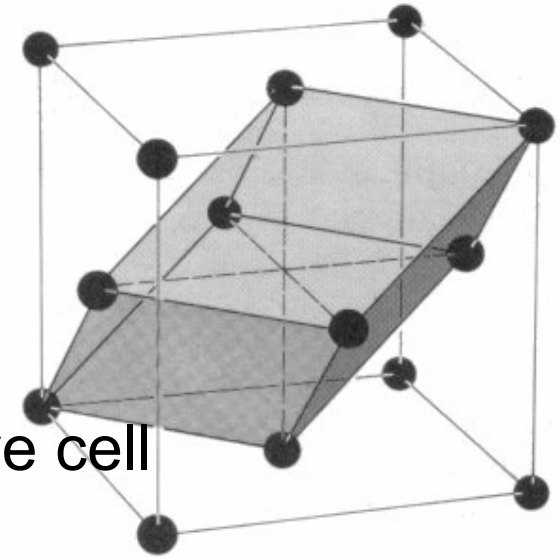


http://cst-www.nrl.navy.mil/bind/kpts/bcc/

Body centered cubic lattice

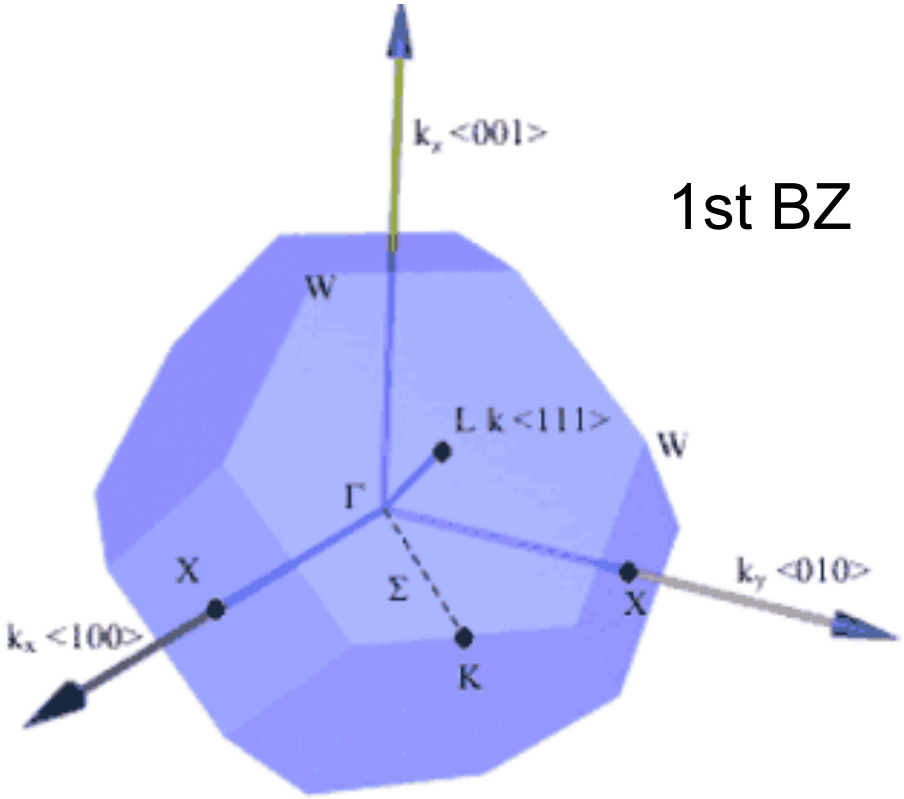


Wigner-Seitz unit cell
(b.t.w = 1st BZ of bcc!)



Primitive cell

$\mathbf{t}_1 = (a/2)\ (0, 1, 1)$
$\mathbf{t}_2 = (a/2)\ (1, 0, 1)$
$\mathbf{t}_3 = (a/2)\ (1, 1, 0)$



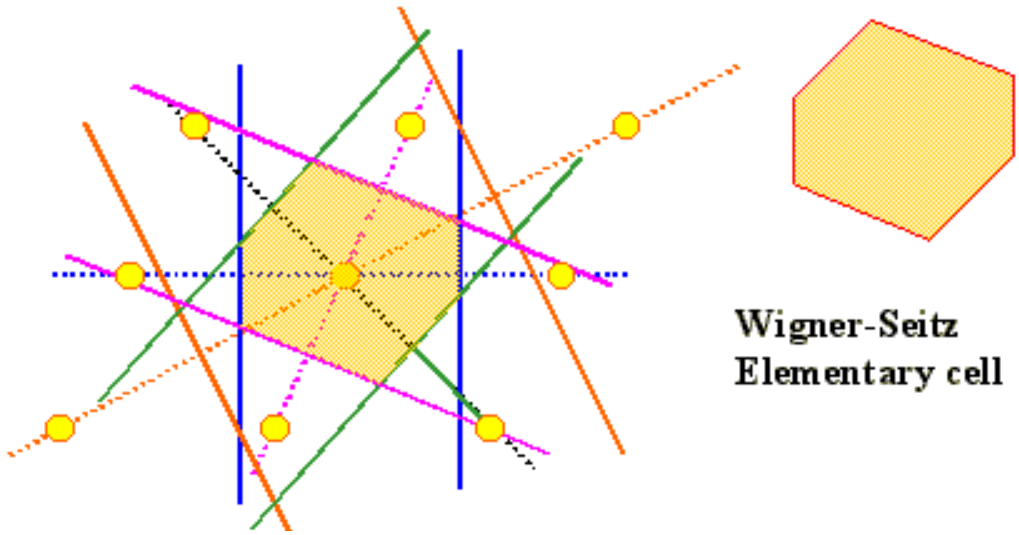
1st BZ

http://britneyspears.ac/physics/crystals/wcrystals.htm

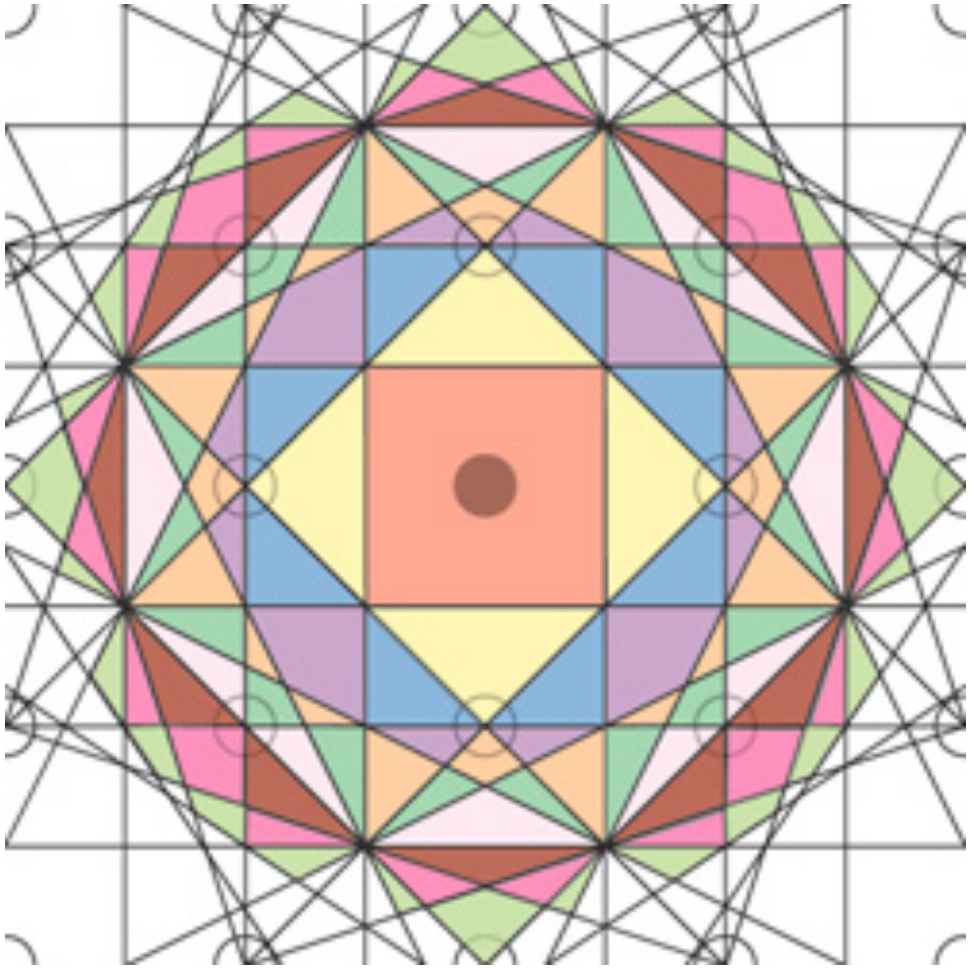
Face centered cubic lattice

Construction of the Wigner-Seitz (WS) unit cell

① Choose a zero point of the lattice.
② Draw lines from zero point to all nearest-neighbor lattice sites
③ Draw lines (planes in 3D), that bisects all lines at a right angle.
④ The smallest area (volume) enclosed by the lines (planes) is the WS cell. If the lattice represents *k*-points, then we call this the first Brillouin zone.
⑤ Draw all the perpendicular bisectors for the 2nd n-n and so on. (solid lines below). The second BZ is found by going from the 1st BZ across one (and only one) of the solid lines.

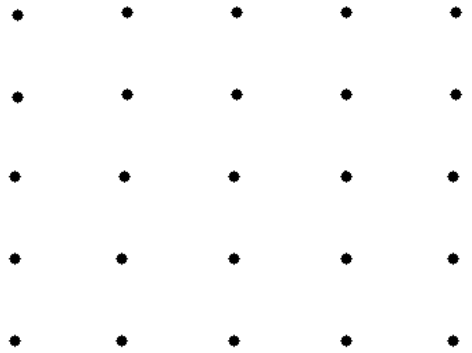


Brillouin zones for square lattice:



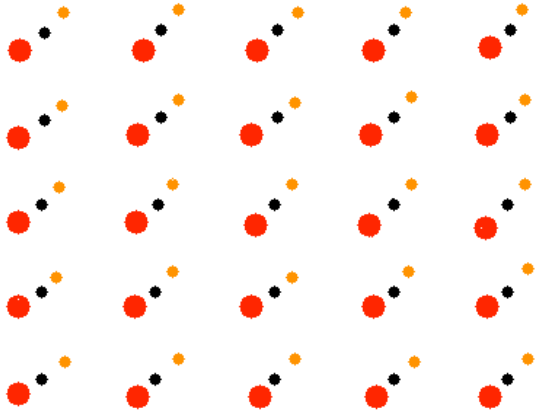
Tutorial at:
http://www.doitpoms.ac.uk/tlplib/brillouin_zones/index.php

Lattice with a basis

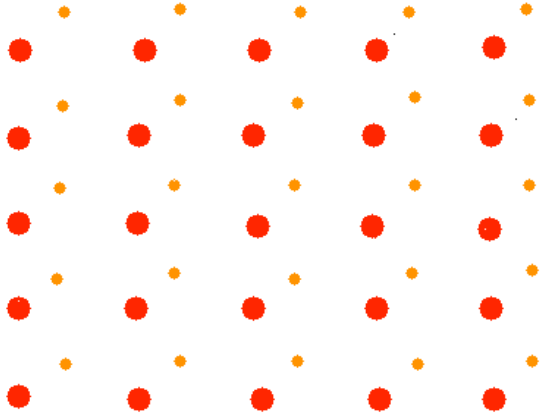


Square lattice

Basis of atoms

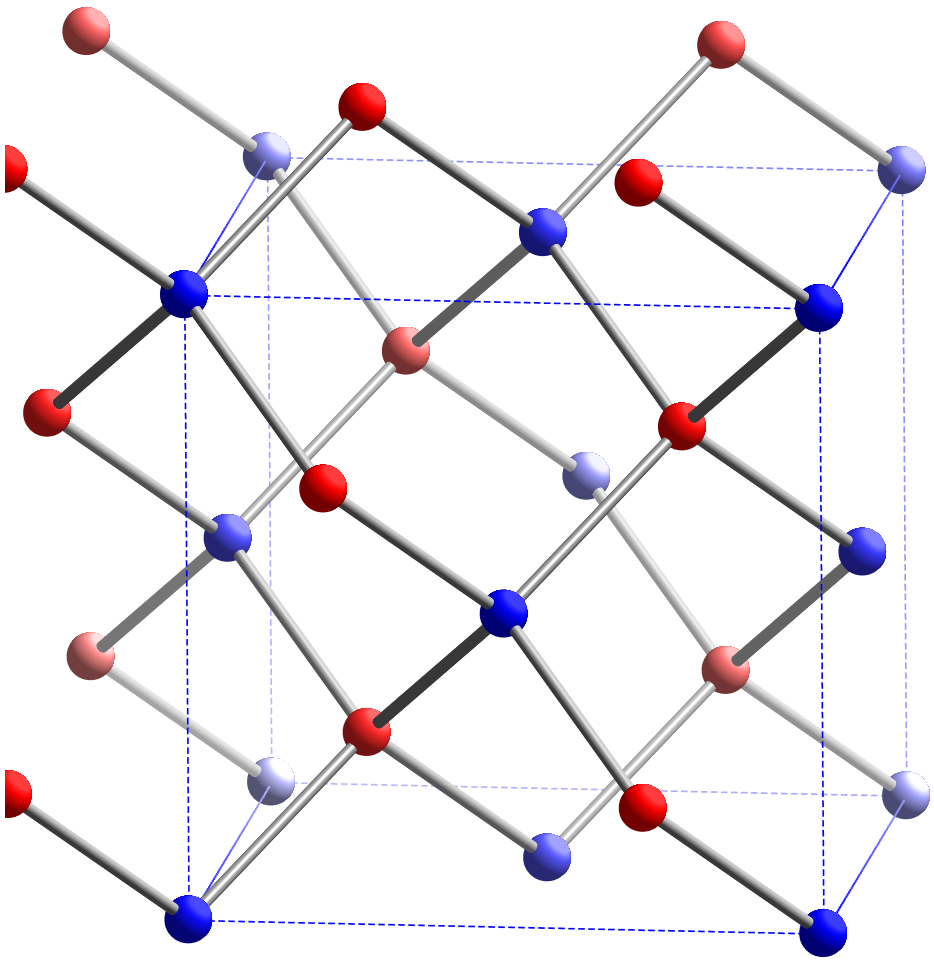


Add together



Just the atoms

Lattice with a basis: Si



FCC lattice
with basis

http://cst-www.nrl.navy.mil/lattice/

Lattice Vectors

$\mathbf{A}_1$ = ½ a **Y** + ½ a **Z**

$\mathbf{A}_2$ = ½ a **X** + ½ a **Z**

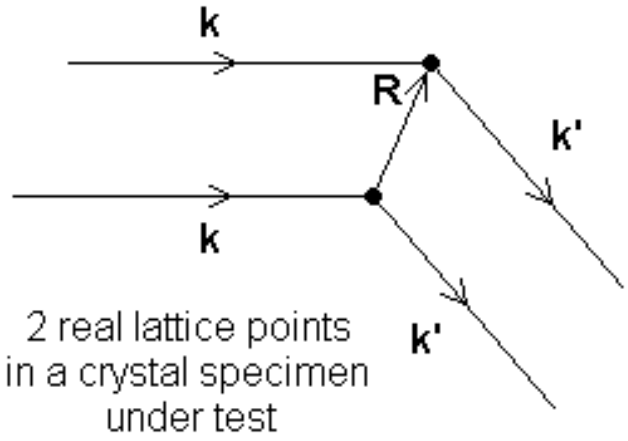
$\mathbf{A}_3$ = ½ a **X** + ½ a **Y**

Basis Vectors

$\mathbf{B}_1$ = -1/8 **A1** - 1/8 **A2** - 1/8 **A3**

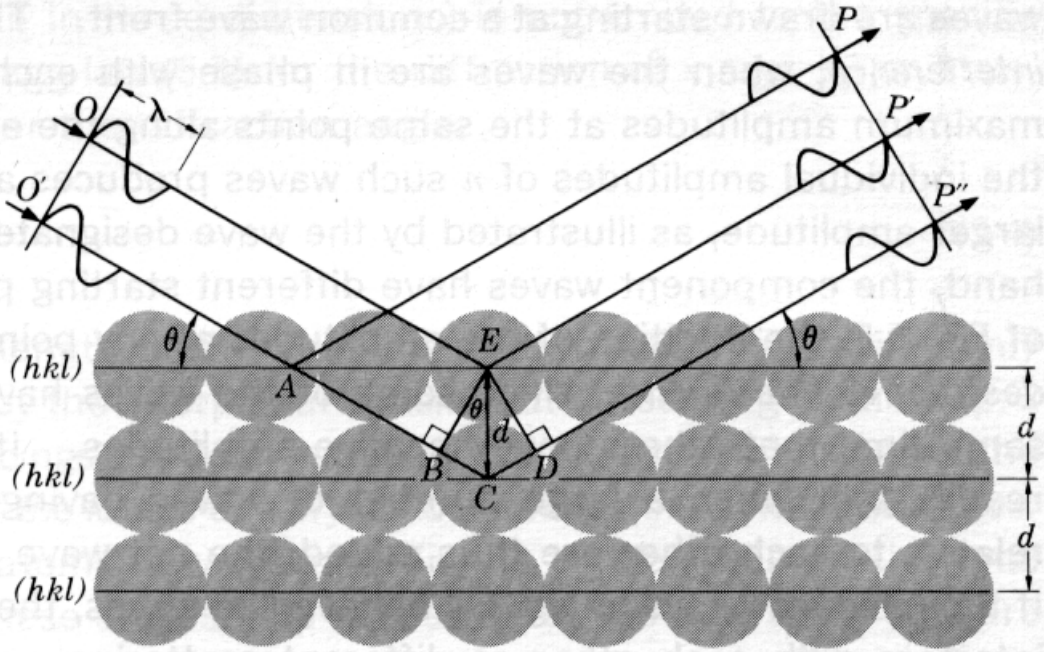
$\mathbf{B}_2$ = 1/8 **A1** + 1/8 **A2** +1/8 **A3**

X-ray diffraction and the reciprocal lattice



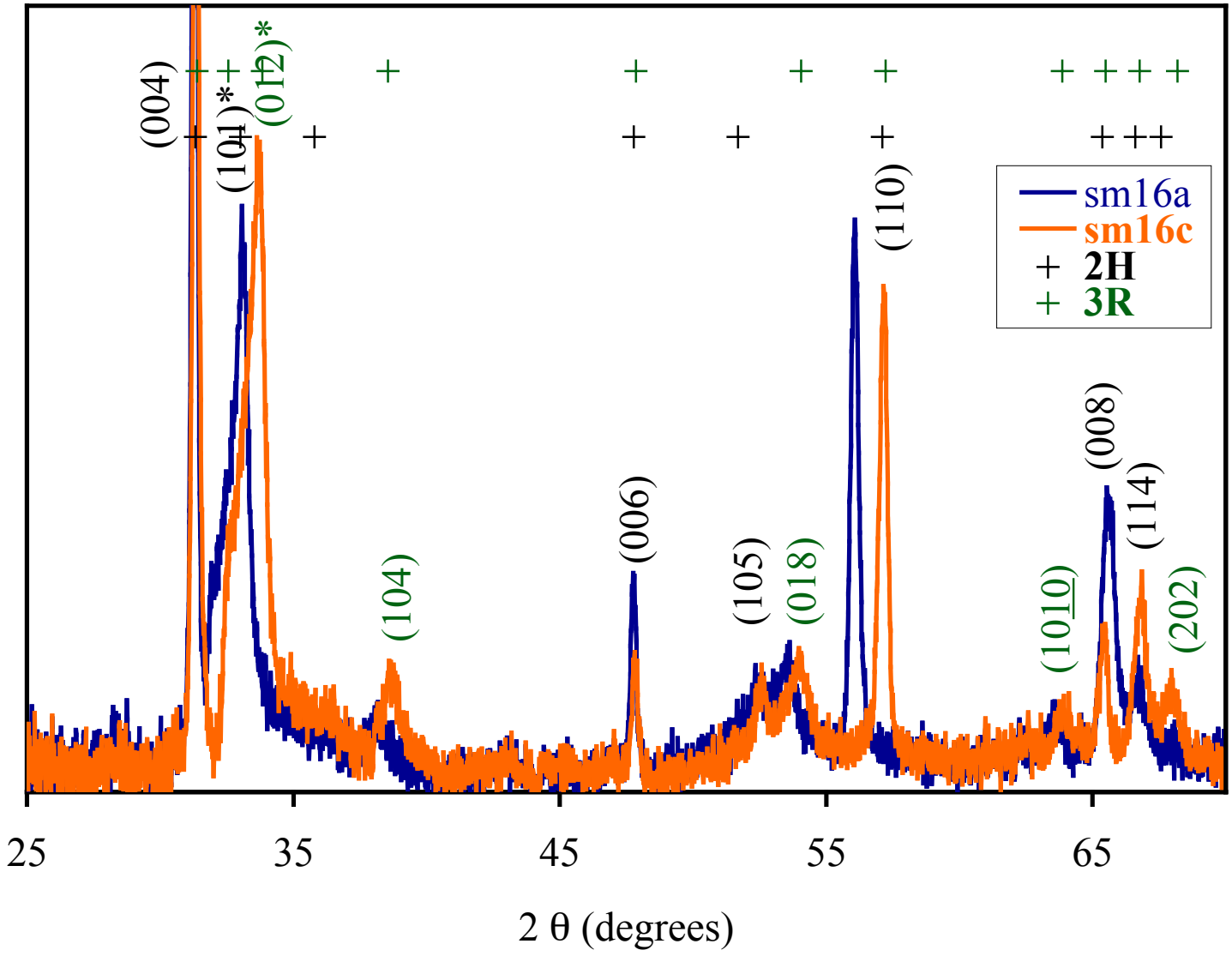
The change in the momentum vector of the X-ray beam is equal to a reciprocal lattice vector (Laue condition. This is equivalent to Bragg's familiar law $n\lambda = 2d \sin\theta$, but is more powerful.

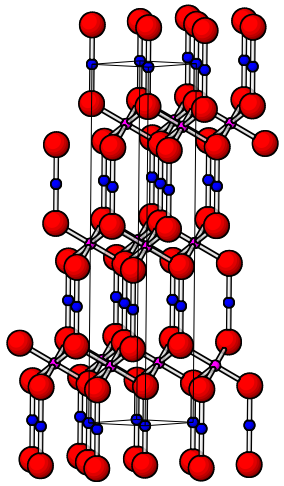
The X-ray diffraction pattern is the Fourier transform (reciprocal lattice) of the real lattice



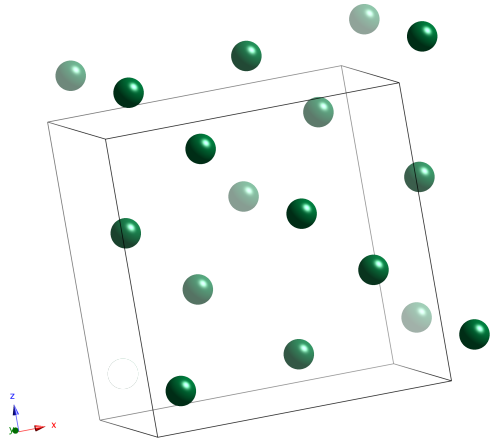
$CuScO_{2+y}$ films

unoxidized ($y \approx 0$) oxygen intercalated ($y \approx 0.5$)





Fd-3m

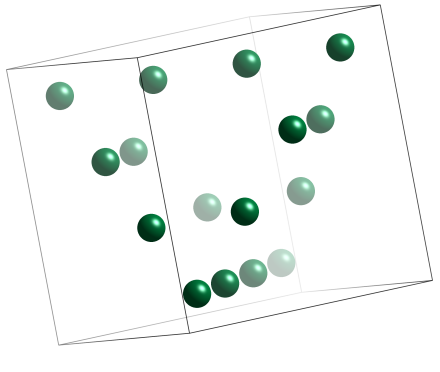


Space group #227 (Si).
Herman-Mauguin symbol is Fd-3m (-3 = 3bar)
F= fcc;
d = glide plane
-3 (3bar) = 3-fold roto-inversion axis
m = mirror plane

Origin 2 ☺
(1/8,1/8,1/8)

We specify some atoms and the symmetry operations ➔
the rest of the atoms positions are then generated.
Choice of origin is important!

Origin 1 ☹
(1/8,1/8,1/8)



CIFs
Crystallographic Information files

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