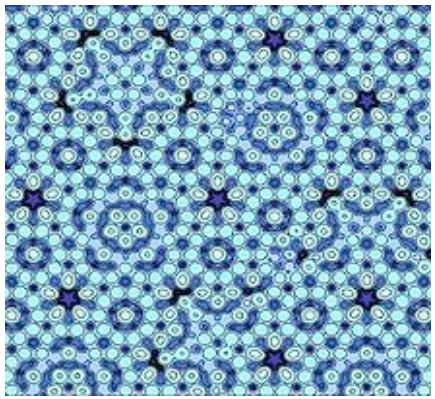
Lecture 2: Crystal Lattices

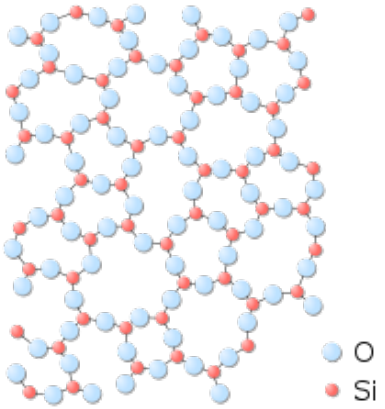
Solids

Crystals -- Atoms are ordered & have periodicity

Quasi - Crystals -- ordered but no periodicity

Amorphous Solids -- not ordered, no periodicity





Introduce “Crystal Lattices”

describe

“Crystal Structures”

Question:

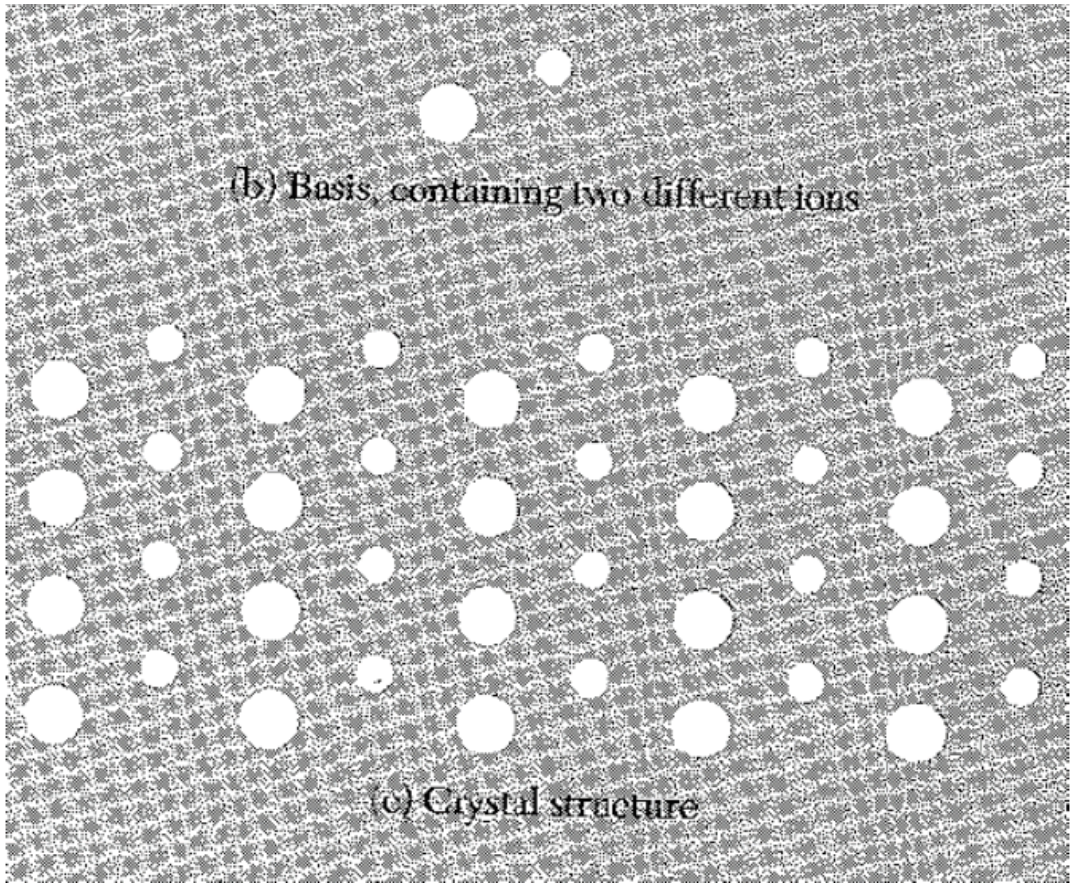
Crystal Lattice = Crystal Structure ?

Basic concepts

- Basis
- Lattice (mathematic constructions)
- Crystal structure = basis + lattice
- Primitive cell = unit cell: one lattice point
- Lattice translation vectors
- Coordination number

Crystal structure: built of atoms
Crystal Lattice: an infinite pattern of points

Basis:
A group of atoms that can be repeated to construct a crystal.



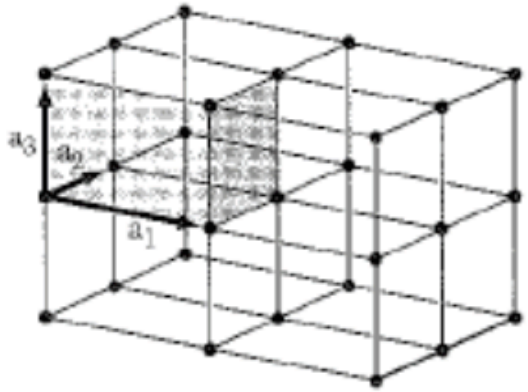
Bravais lattice:

The distinct lattice types which can fill the whole space when repeated . The lattice can therefore be generated by three unit vectors, $\mathbf{a_1}$, $\mathbf{a_2}$ and $\mathbf{a_3}$ and a set of integers k, l and m so that each lattice point, identified by a vector **r**, can be obtained from:

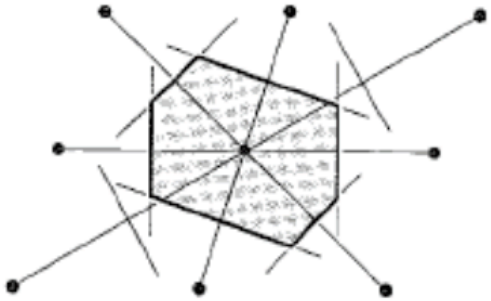
$$\mathbf{r} = k\,\mathbf{a_1} + l\,\mathbf{a_2} + m\,\mathbf{a_3}$$

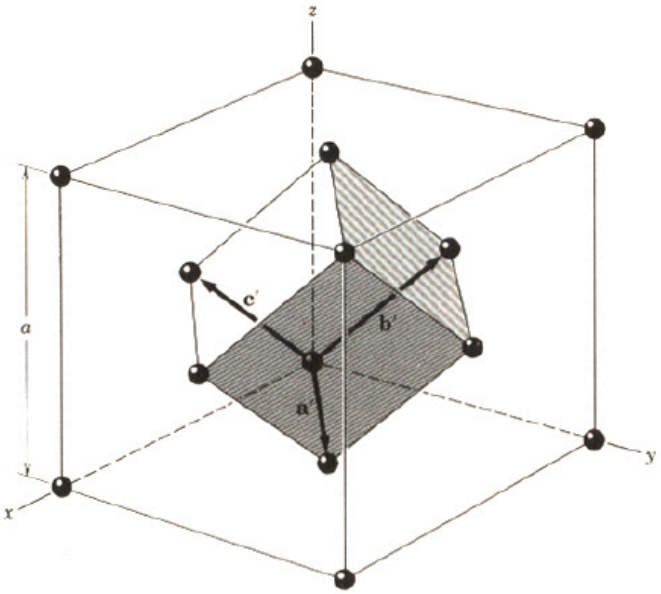
Lattice translation vectors: $\mathbf{a_1}$, $\mathbf{a_2}$ and $\mathbf{a_3}$

Primitive cell:



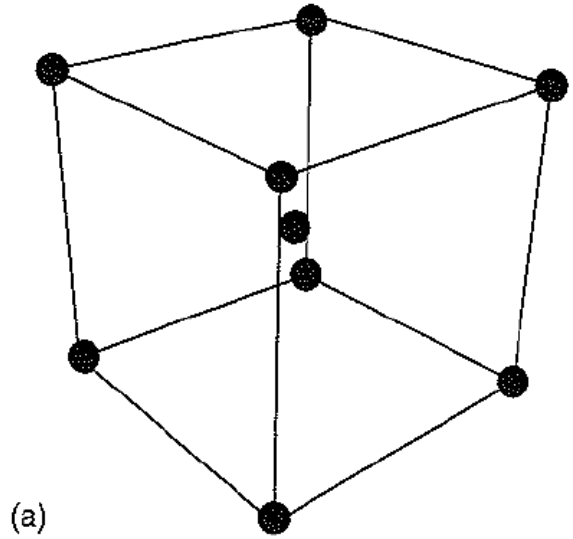
Wigner-Seitz cell:

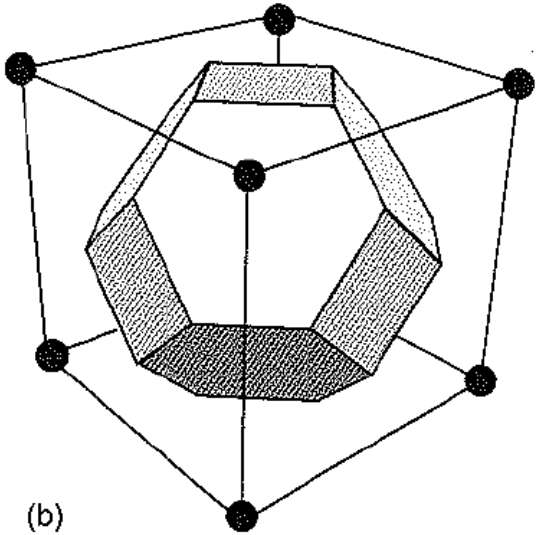


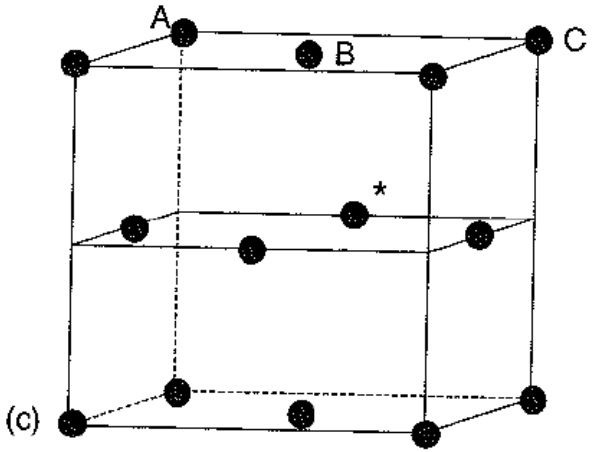


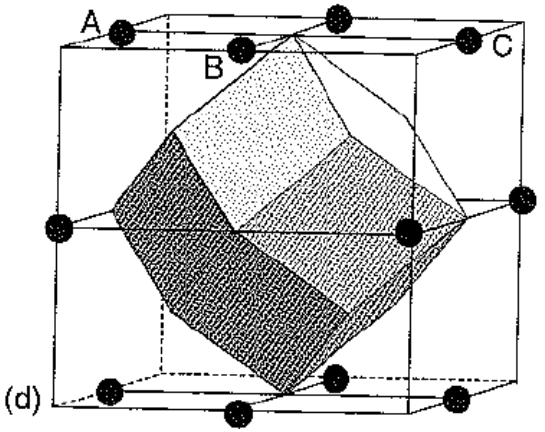
Coordination number:

Primitive cell ⟷ Wigner-Seize cell







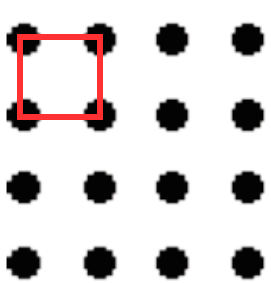


Two-dimensional Lattice Types

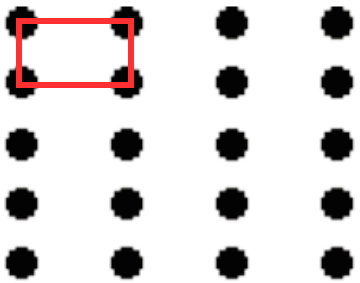
5 Bravais lattice:

- $a_1 = a_2$, $\varphi = 90°$
- $a_1 = a_2$, $\varphi = 120°$ (hexagonal lattice)
- $a_1 \neq a_2$, $\varphi = 90°$
- $a_1 \neq a_2$, $\varphi = 90°$ (centered)
- $a_1 \neq a_2$, $\varphi \neq 90°$

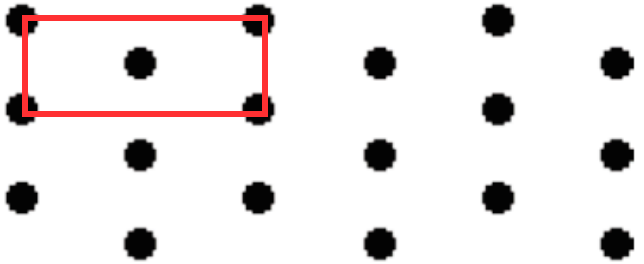
Two-dimensional Lattice Types



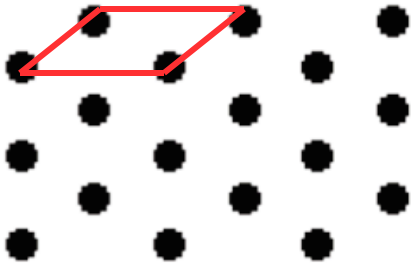
Square
(tp)



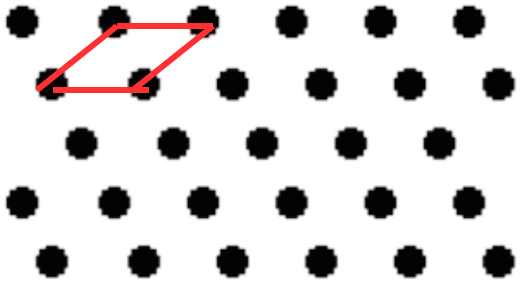
Rectangular
(op)



Centered Rectangular
(oc)



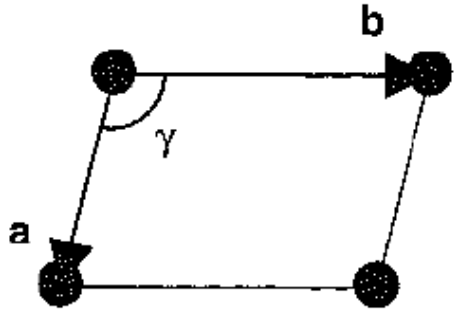
Hexagonal
(hp)



Oblique
(mp)

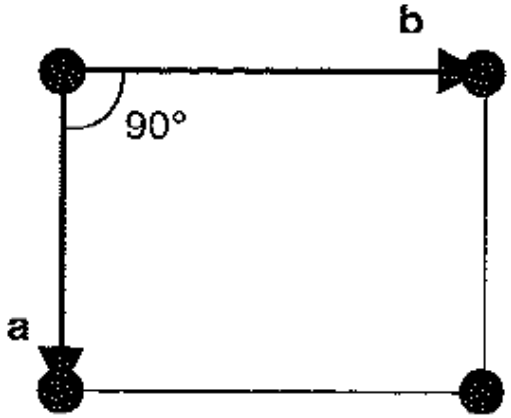
Oblique primitive (*mp*)

(a)



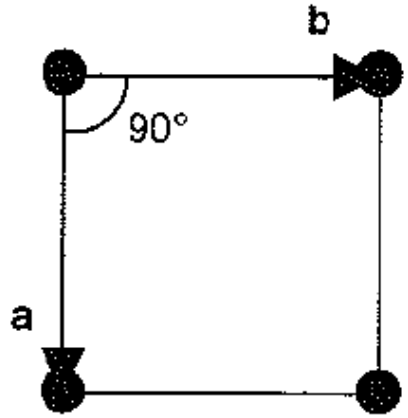
Rectangular primitive (*op*)

(b)



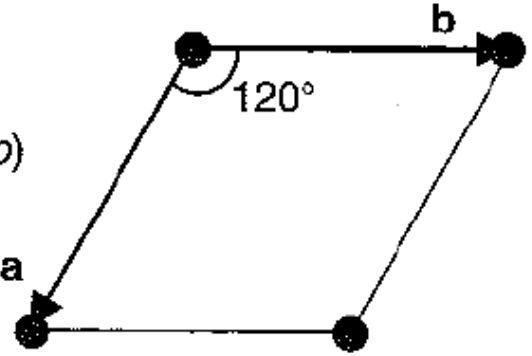
Square primitive (*tp*)

(c)



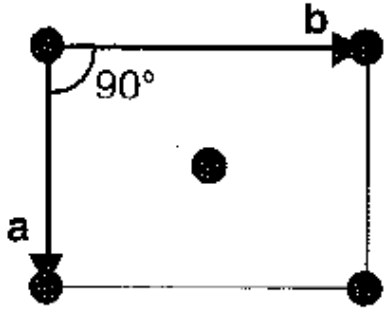
Hexagonal primitive (*hp*)

(d)

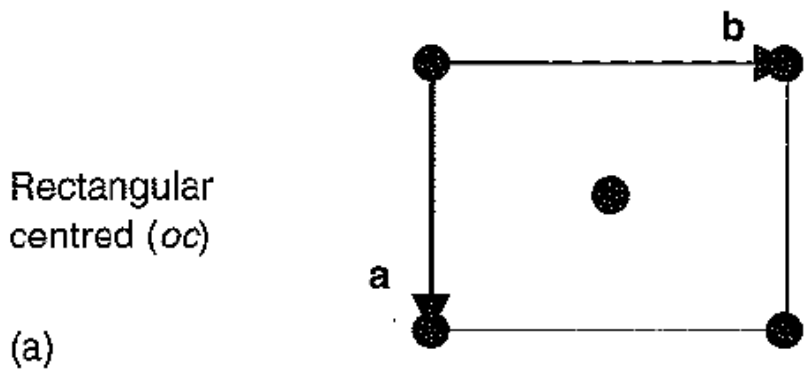


Rectangular centred (*oc*)

(e)

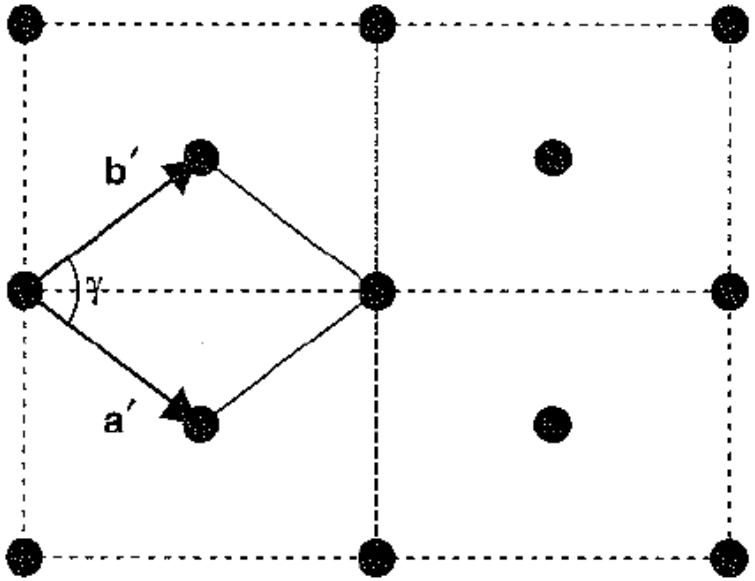


Is this a primitive cell?



Rectangular centred (*oc*)

(a)



Rhombic primitive (*rp*)

(b)

Answer:

No. A primitive cell can only have one point!

What is the unit cell of a System with pentagonal symmetry?

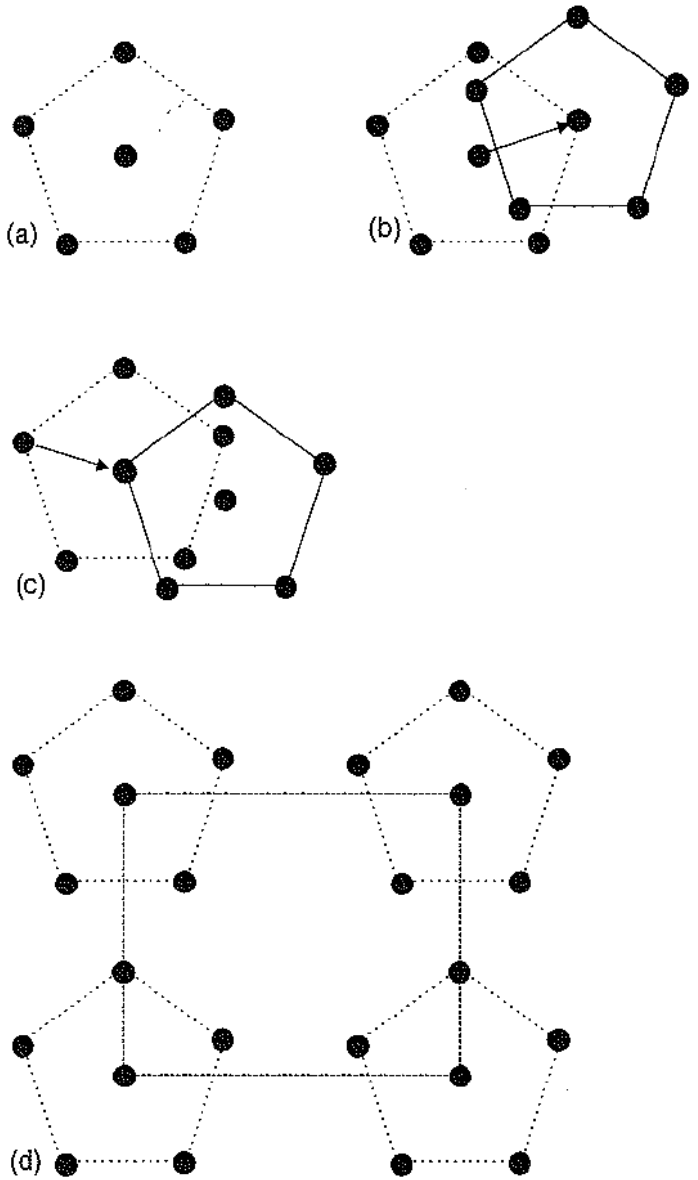


Table 2.2 Bravais lattices

Crystal system	Lattice symbol	Lattice parameters
Triclinic	*aP*	$a \neq b \neq c$, $\alpha \neq 90°$, $\beta \neq 90°$, $\gamma \neq 90°$;
Monoclinic primitive	*mP*	$a \neq b \neq c$, $\alpha = 90°$, $\beta \neq 90°$, $\gamma = 90°$;
Monoclinic centred	*mC*	
Orthorhombic primitive	*oP*	$a \neq b \neq c$, $\alpha = \beta = \gamma = 90°$
Orthorhombic *C*-face-centred	*oC*	
Orthorhombic body-centred	*oI*	
Orthorhombic face-centred	*oF*	
Tetragonal primitive	*tP*	$a = b \neq c$, $\alpha = \beta = \gamma = 90°$
Tetragonal body-centred	*tI*	
Trigonal (Rhombohedral)	*hR*	$a = b = c$, $\alpha = \beta = \gamma$ (primitive cell); $a' = b' \neq c'$, $\alpha' = \beta' = 90°$, $\gamma' = 120°$ (hexagonal cell)
Hexagonal primitive	*hP*	$a = b \neq c$, $\alpha = \beta = 90°$, $\gamma = 120°$
Cubic primitive	*cP*	$a = b = c$, $\alpha = \beta = \gamma = 90°$
Cubic body-centred	*cI*	
Cubic face-centred	*cF*	

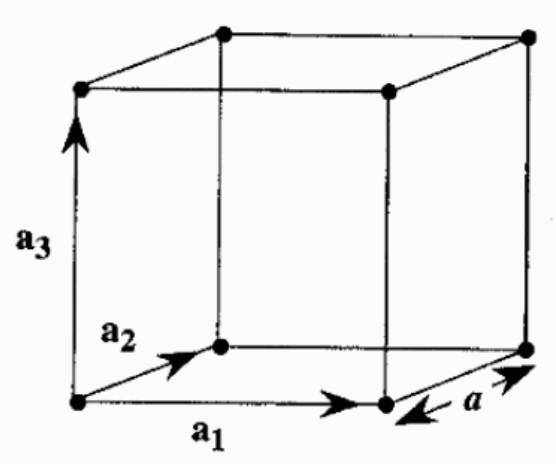
Three-dimensional Lattice Types

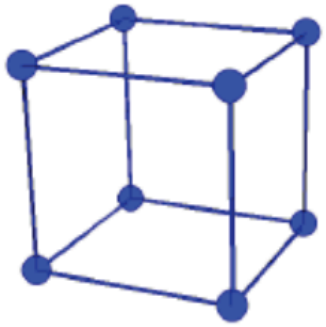
- Cubic:

$a_1 = a_2 = a_3$, $\alpha = \beta = \gamma = 90°$

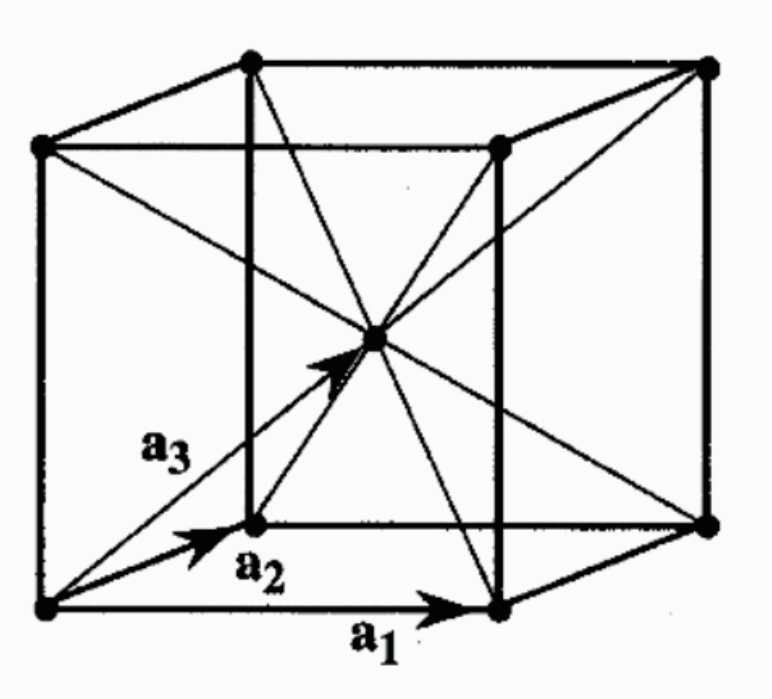
Simple cubic
Body-centered cubic
Face-center cubic

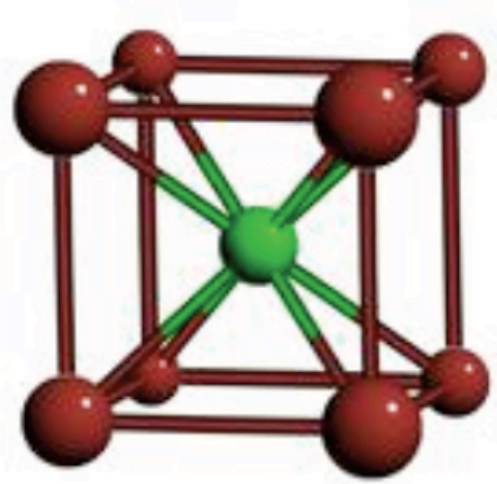
Simple Cubic





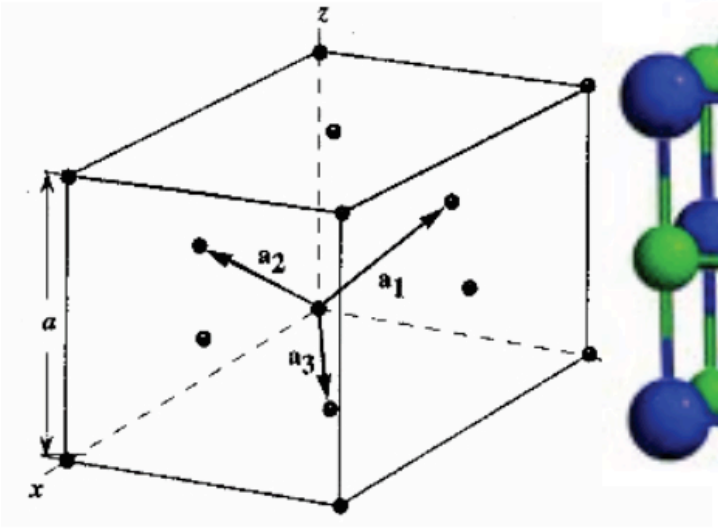
Body-Centered Cubic

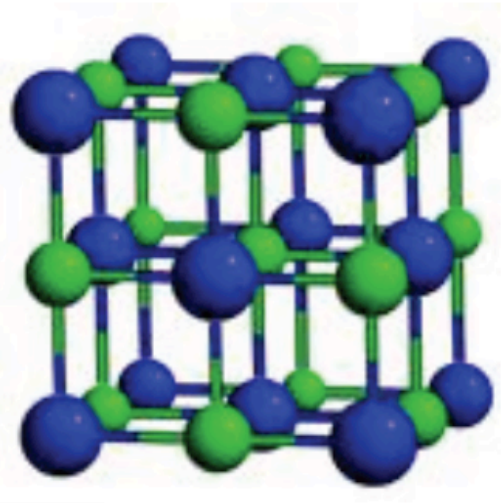




Face-Centered Cubic

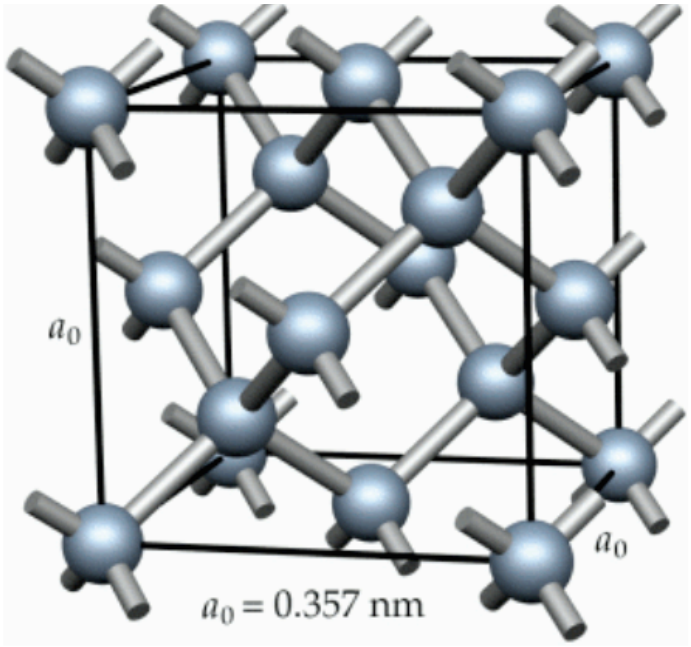
Basis: (0,0,0) and (1/2,0,0)





NaCl

Basis: (0,0,0) and (1/4,1/4,1/4)

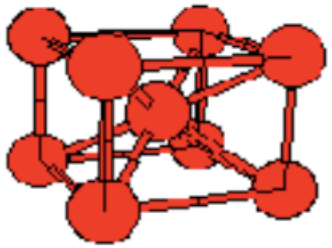


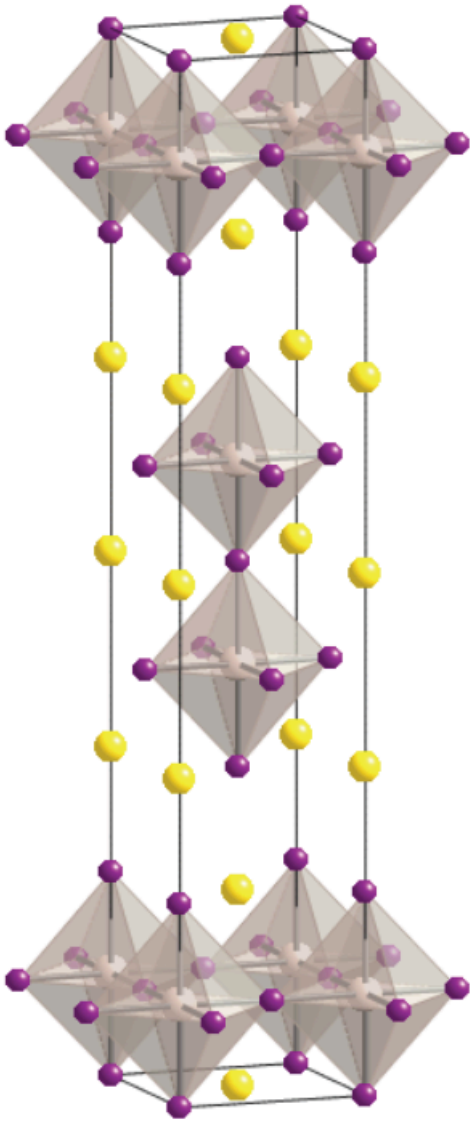
Diamond

Three-dimensional Lattice Types

- Tetragonal:

$a_1 = a_2 \neq a_3$, $\alpha = \beta = \gamma = 90°$

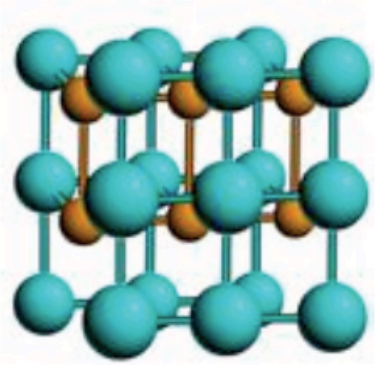


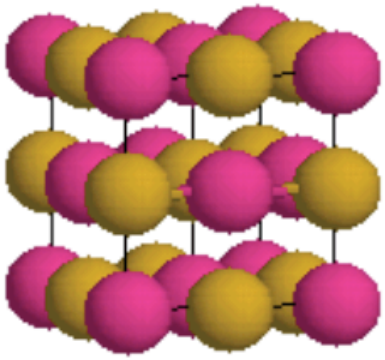


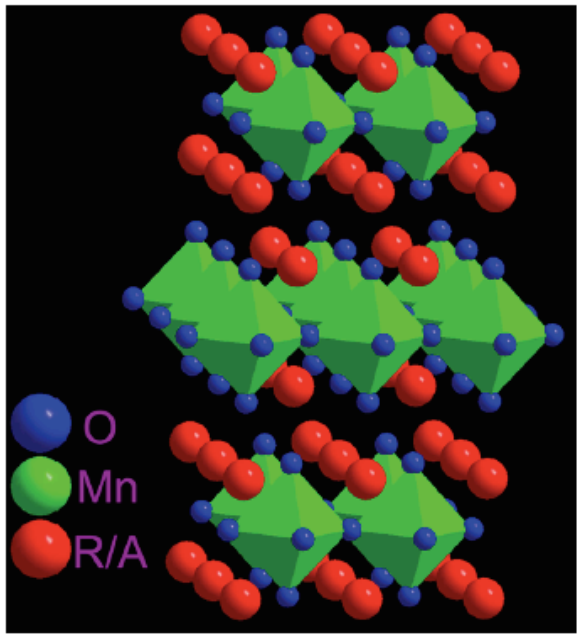
Three-dimensional Lattice Types

- Orthorhombic:

$a_1 \neq a_2 \neq a_3$, $\alpha = \beta = \gamma = 90°$



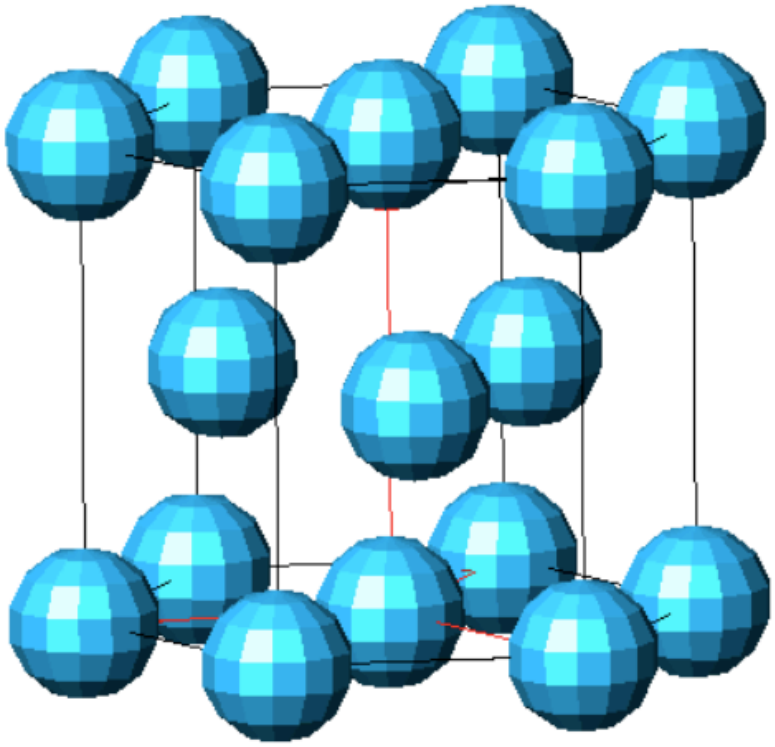




Three-dimensional Lattice Types

- Hexagonal:

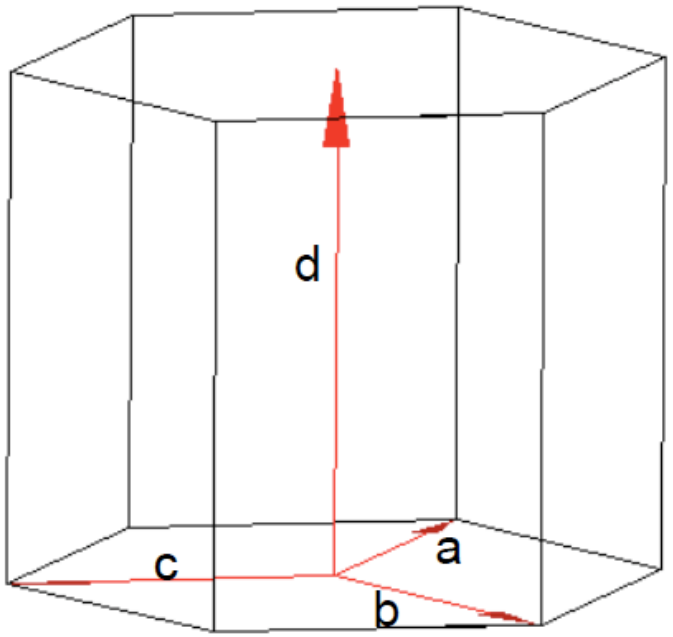
$$a_1 = a_2 \neq a_3,\ \alpha = \beta = 90°,\ \gamma = 120°$$



A Plane

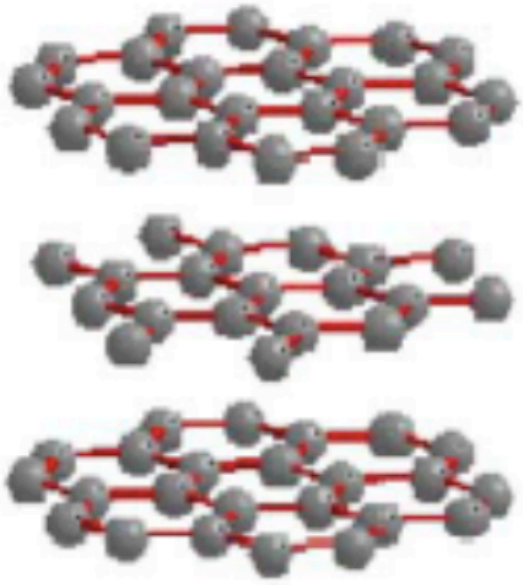
B Plane

A Plane

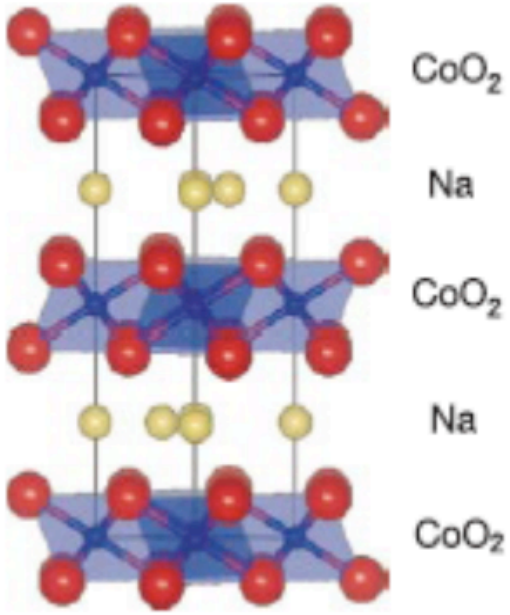


HCP Structure: Stacking sequence ABAB

Hexagonal Structure



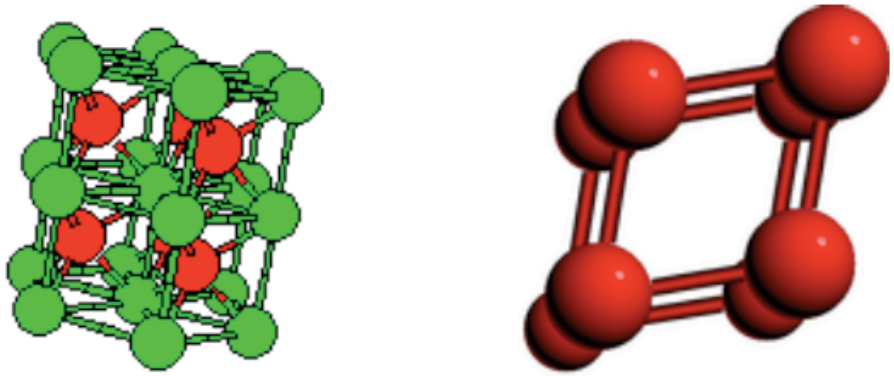
graphite



Three-dimensional Lattice Types

- Trigonal:

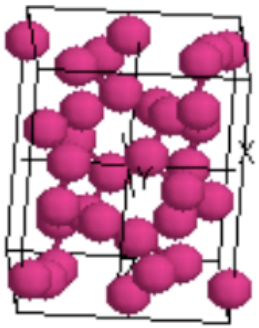
$a_1 = a_2 = a_3$, $\alpha = \beta = \gamma < 120°, \neq 90°$,

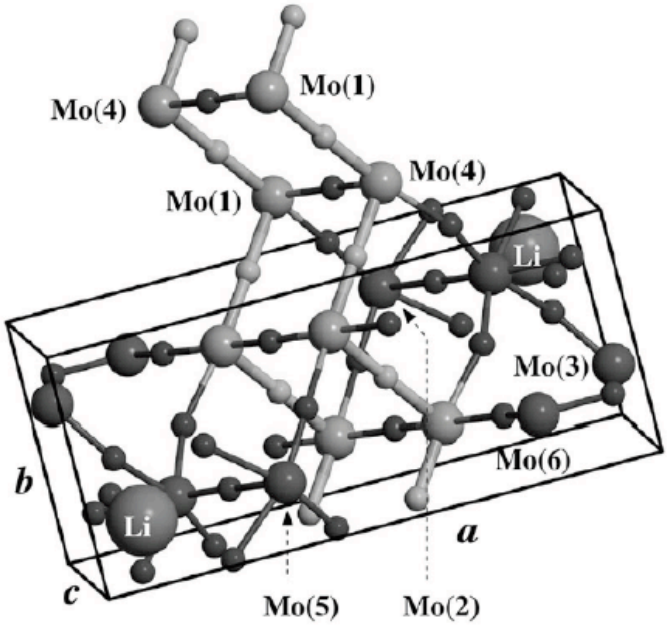


Three-dimensional Lattice Types

- Monoclinic:

$a_1 \neq a_2 \neq a_3$, $\alpha = \gamma = 90°$, $\beta \neq 90°$,





Three-dimensional Lattice Types

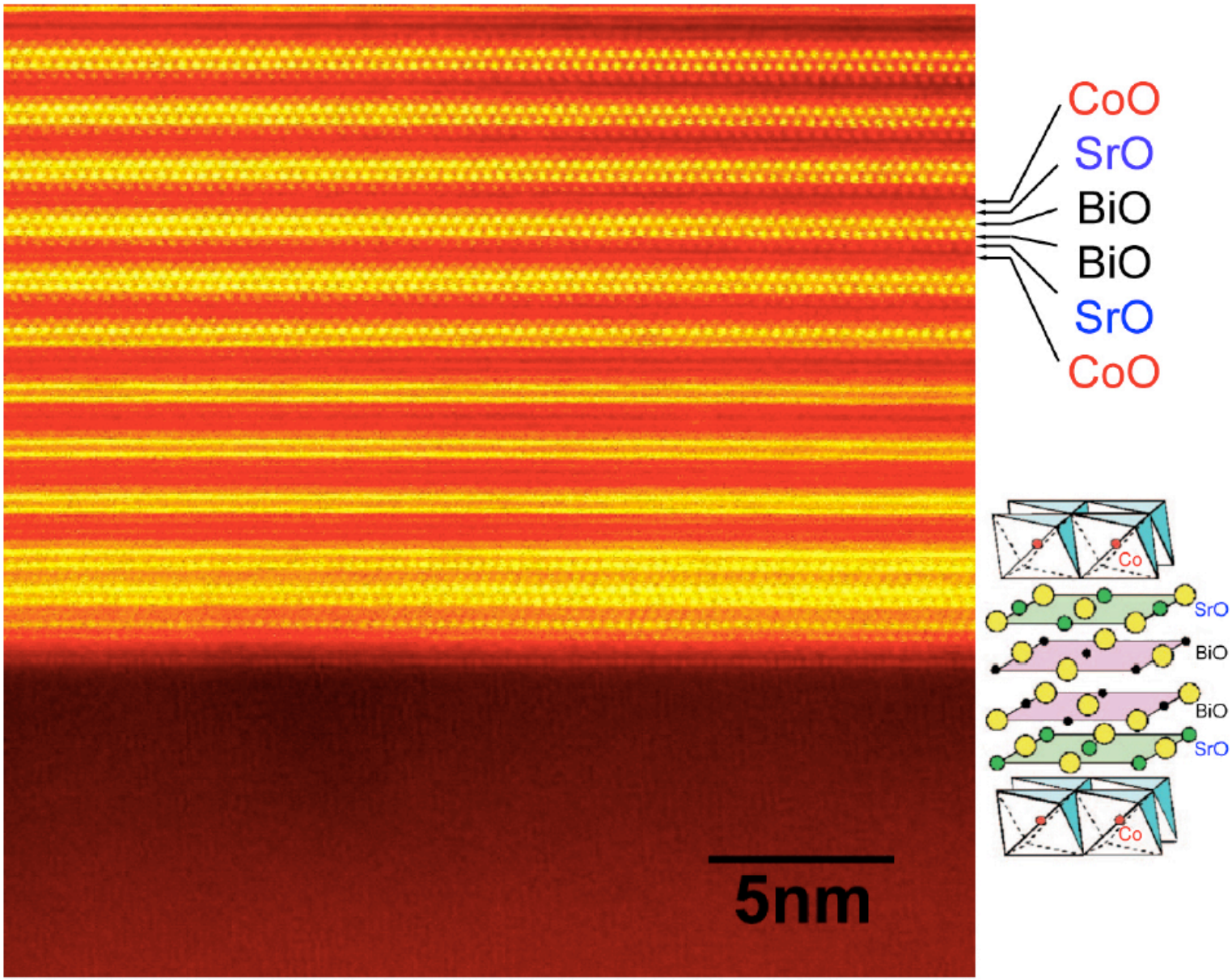
- Triclinic:

$a_1 \neq a_2 \neq a_3$, $\alpha \neq \beta \neq \gamma$

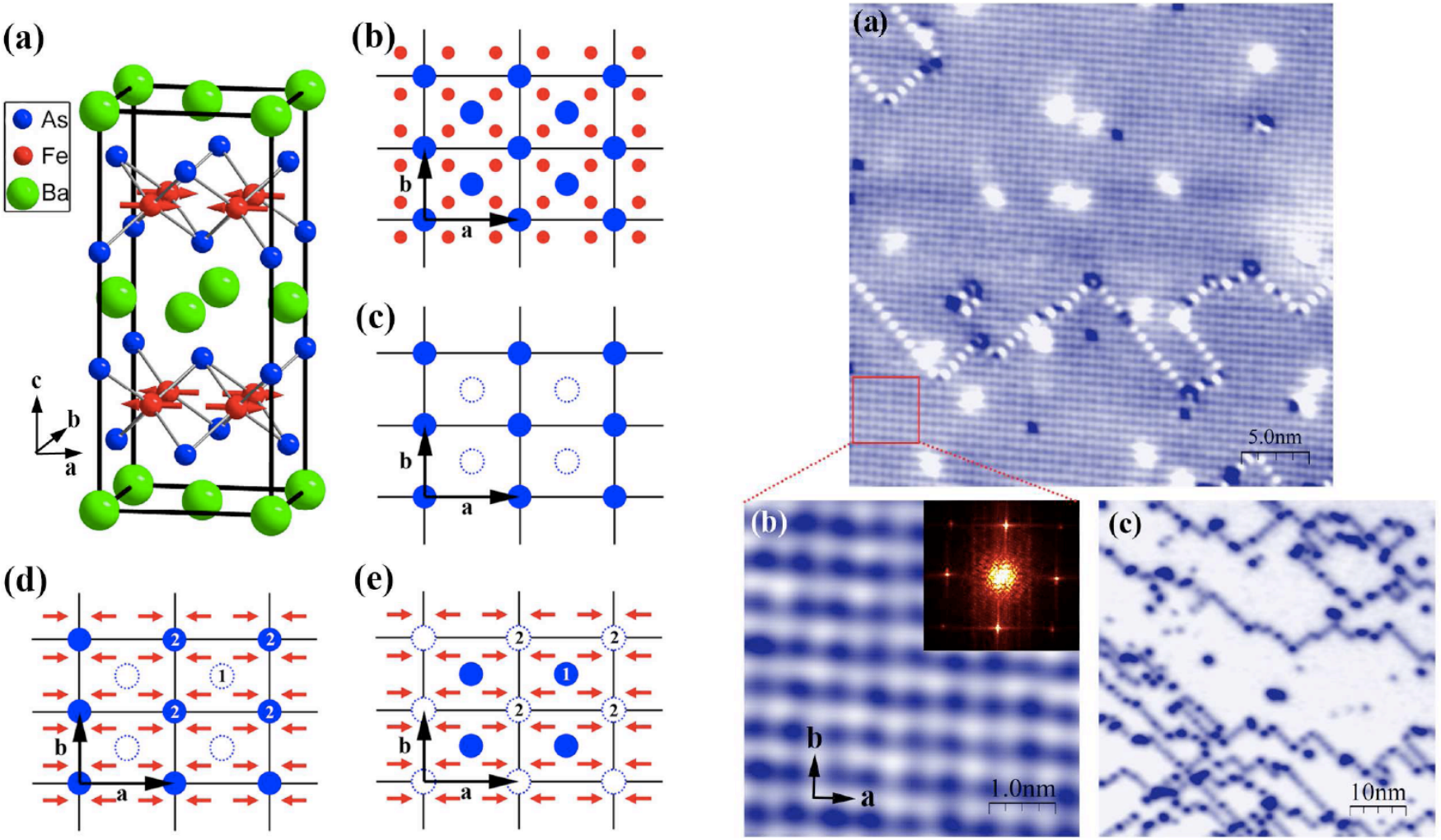
Direct Imaging of Atomic Structure

- Transmission electron microscopy
- Scanning tunneling microscopy
  (reflected by local electronic density of states – surface only)

TEM



STM



Homework today (due on Sept. 2, 2010)

Problems 1 and 5 in page 82 (Ashcroft/Mermin)

The Reciprocal Lattice

A set of wave vectors **K** that ensure

$$e^{i\mathbf{K}\bullet\mathbf{R}} = 1$$

Direct lattice (Bravais lattice): $\mathbf{R} = n_1\mathbf{a_1} + n_2\mathbf{a_2} + n_3\mathbf{a_3}$

Reciprocal lattice: $\mathbf{K} = k_1\mathbf{b_1} + k_2\mathbf{b_2} + k_3\mathbf{b_3}$

Direct lattice (Bravais lattice): $\mathbf{R} = n_1\mathbf{a_1}+n_2\mathbf{a_2}+n_3\mathbf{a_3}$

Reciprocal lattice: $\mathbf{K} = k_1\mathbf{b_1}+k_2\mathbf{b_2}+k_3\mathbf{b_3}$

$$\boldsymbol{b}_1 = 2\pi \frac{\boldsymbol{a}_2 \times \boldsymbol{a}_3}{\boldsymbol{a}_1 \bullet \left(\boldsymbol{a}_2 \times \boldsymbol{a}_3\right)}$$

$$\boldsymbol{b}_2 = 2\pi \frac{\boldsymbol{a}_3 \times \boldsymbol{a}_1}{\boldsymbol{a}_1 \bullet \left(\boldsymbol{a}_2 \times \boldsymbol{a}_3\right)}$$

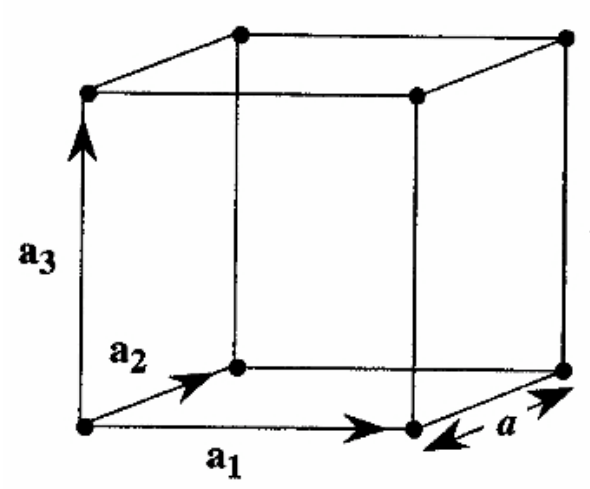
$$\boldsymbol{b}_3 = 2\pi \frac{\boldsymbol{a}_1 \times \boldsymbol{a}_2}{\boldsymbol{a}_1 \bullet \left(\boldsymbol{a}_2 \times \boldsymbol{a}_3\right)}$$

$$\boldsymbol{b}_i \bullet \boldsymbol{a}_j = 2\pi\delta_{ij}$$

	volume
Direct lattice (Bravais lattice):	v
Reciprocal lattice:	$(2\pi)^3/v$

Reciprocal lattice itself is also a Bravais lattice

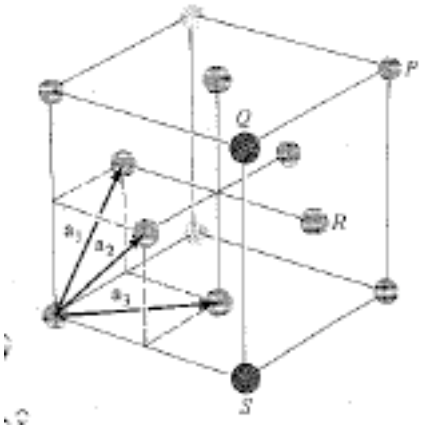
Simple cubic Bravais lattice:



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

$\mathbf{b}_1 = (2\pi/a)\mathbf{x}$, $\mathbf{b}_2 = (2\pi/a)\,\mathbf{y}$, $\mathbf{b}_3 = (2\pi/a)\mathbf{z}$

Face-centered cubic Bravais lattice:



$\mathbf{a}_1 = (a/2)(\mathbf{y}+\mathbf{z})$, $\mathbf{a}_2 = (a/2)(\mathbf{z}+\mathbf{x})$, $\mathbf{a}_3 = (a/2)(\mathbf{x}+\mathbf{y})$

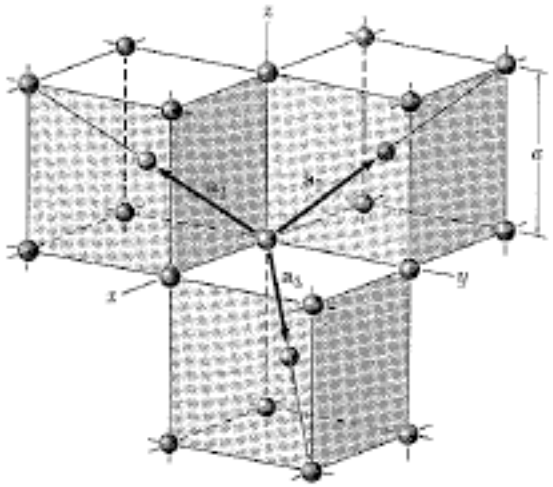
$\mathbf{b}_1 = (4\pi/a)[(1/2)(\mathbf{y}+\mathbf{z}-\mathbf{x})]$
$\mathbf{b}_2 = (4\pi/a)[(1/2)(\mathbf{z}+\mathbf{x}-\mathbf{y})]$
$\mathbf{b}_3 = (4\pi/a)[(1/2)(\mathbf{x}+\mathbf{y}-\mathbf{z})]$

Face-centered cubic
reciprocal lattice:

$\mathbf{b_1} = (4\pi/a)[(1/2)(\mathbf{y+z-x})]$
$\mathbf{b_2} = (4\pi/a)[(1/2)(\mathbf{z+x-y})]$
$\mathbf{b_3} = (4\pi/a)[(1/2)(\mathbf{x+y-z})]$

Body-centered cubic
Bravais lattice

$\mathbf{a_1} = (a/2)(\mathbf{y+z-x})]$
$\mathbf{a_2} = (a/2)(\mathbf{z+x-y})]$
$\mathbf{a_3} = (a/2)(\mathbf{x+y-z})]$

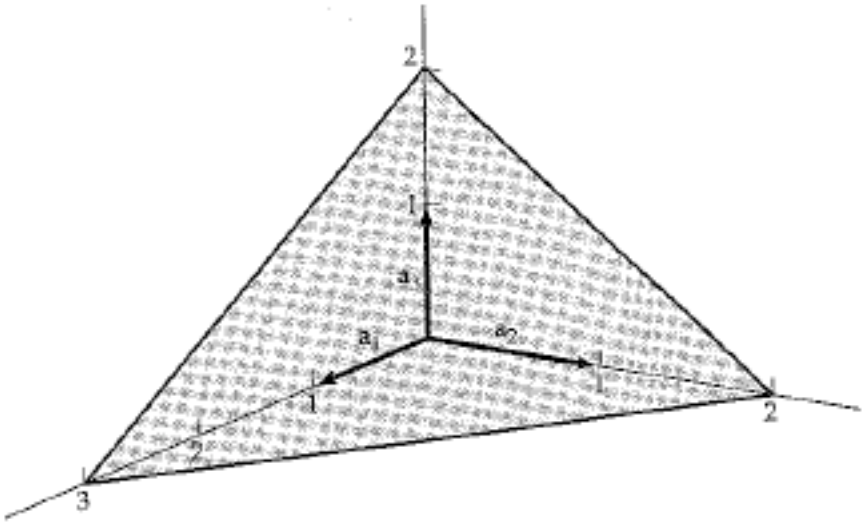


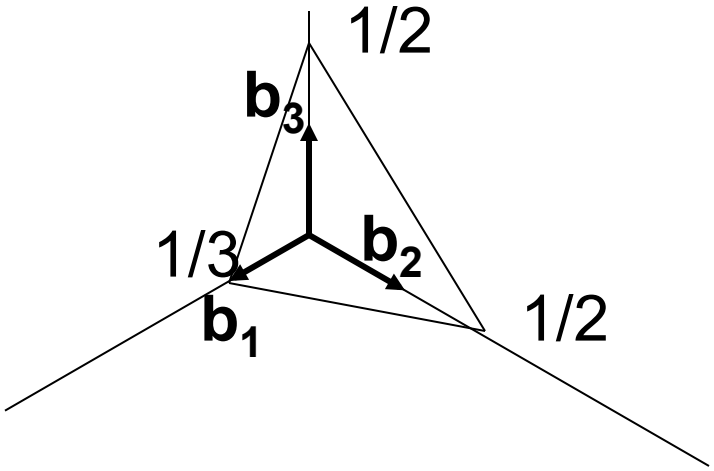
Lattice Planes

- Any lattice plane that contains ≥ 3 non-collinear Bravais lattice points
- Separated by distance d
- Perpendicular to its reciprocal lattice vector
- Not unique

Application:
Name Lattice Planes - Miller Indices

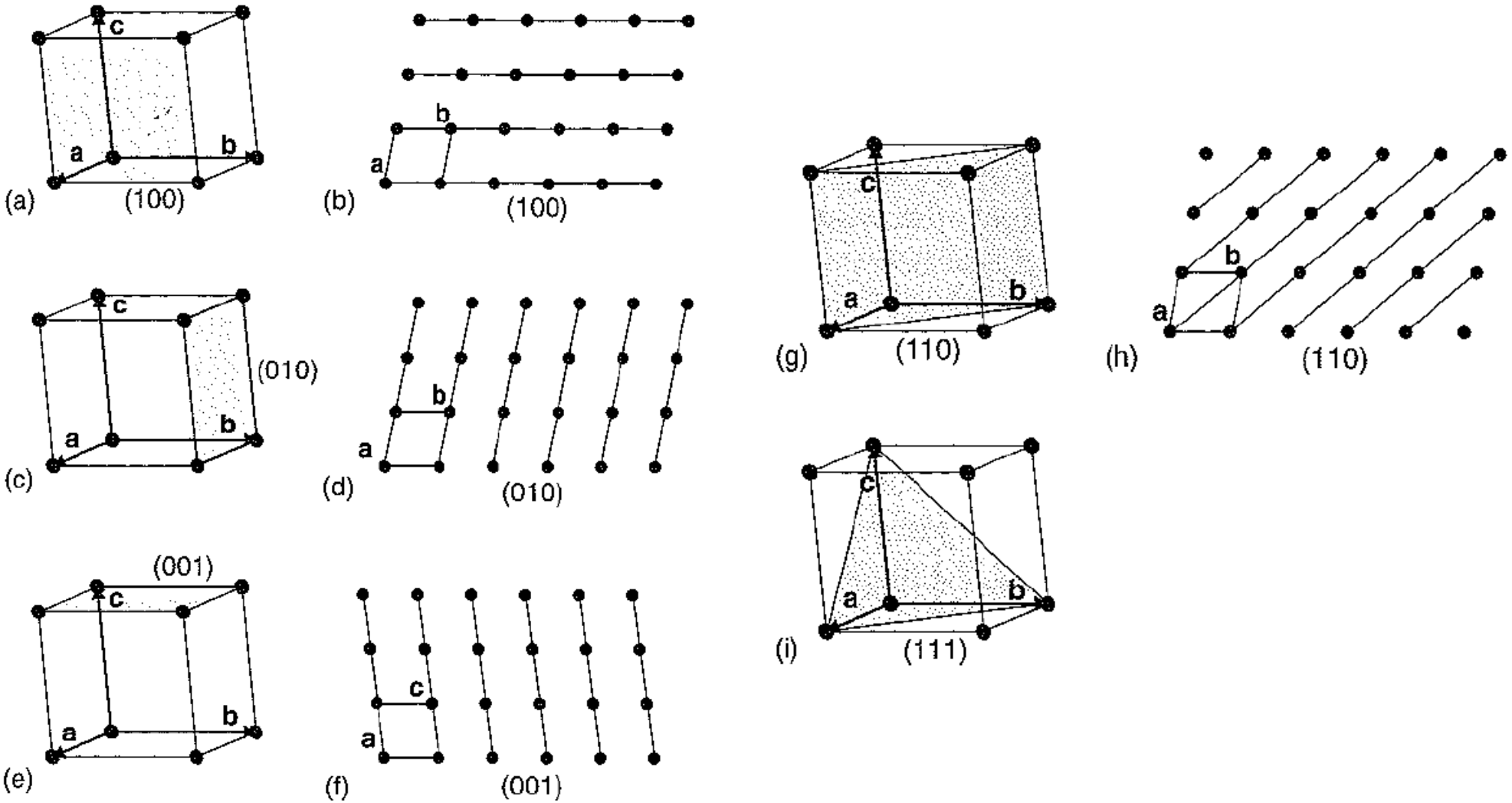
Direct lattice

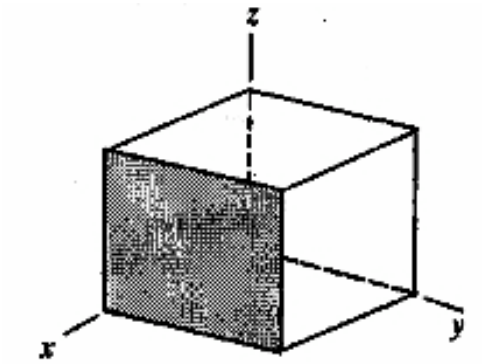


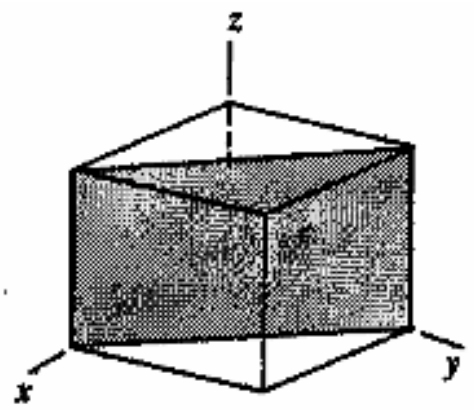


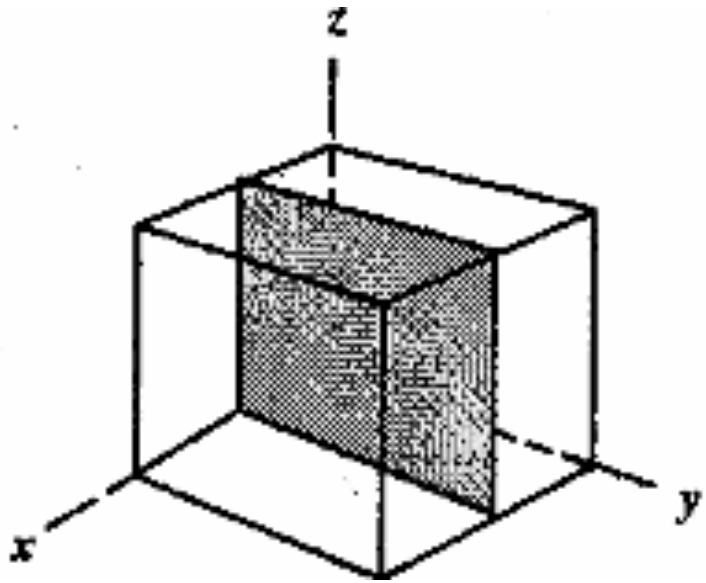
The smallest three integers having the same ratio as
1/3 : 1/2 : 1/2 = 2 : 3 : 3

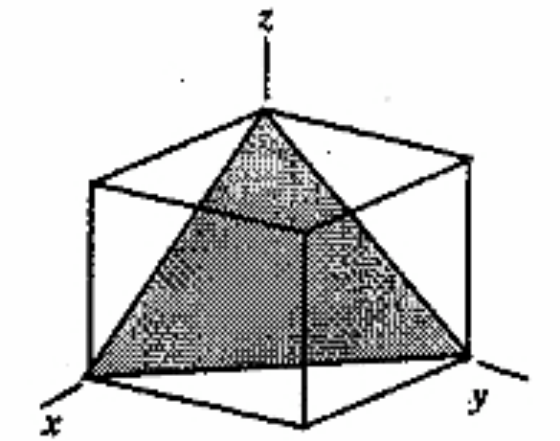
The plane is called (233) plane - Miller Indices

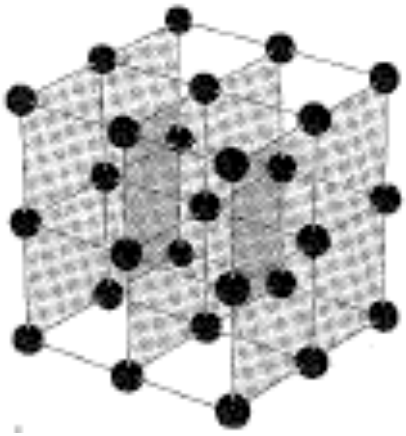

c
a
b
(a)
(100)
b
a
(b)
(100)
c
(010)
a
b
(c)
b
a
(d)
(010)
(001)
c
a
b
(e)
c
a
(f)
(001)
c
a
b
(g)
(110)
b
a
(h)
(110)
c
a
b
(i)
(111)


z
x
y


z
x
y


z
x
y


z
x
y



The end of lecture today!