

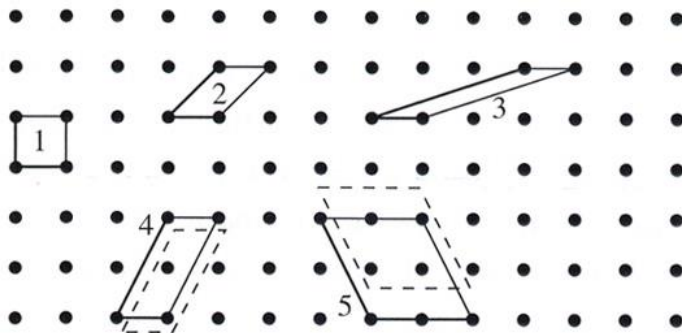
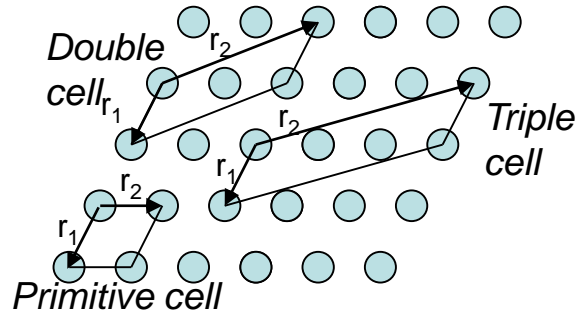


Types of Lattices

Types of Lattices

Lattices are either:

1. Primitive (or Simple): one lattice point per unit cell.
2. Non-primitive, (or Multiple) e.g. double, triple, etc.: more than one lattice point per unit cell.



•When repeated by successive translations reproduce periodic pattern.

•Multiple cells are usually selected to make obvious the higher symmetry (usually rotational symmetry) that is possessed by the lattice, which may not be immediately evident from primitive cell.

“Lattice points are arranged such that each has identical surroundings”

When we arrange lattice points to fill space in the most efficient manner while maintaining the requirement concerning identical surroundings



14 Bravais Lattices

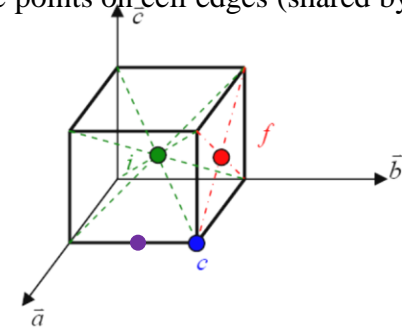
First we must know the number of lattice points within a unit cell

The number of lattice points is given by the equation:

$$N = N_i + \frac{N_f}{2} + \frac{N_c}{8} + \frac{N_e}{4}$$

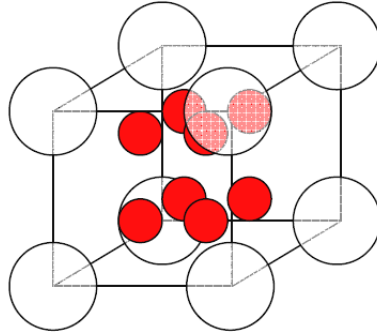
- N_i = number of lattice points in cell interior (belong to 1 cell)
- N_f = number of lattice points on cell faces (shared by 2 cells)
- N_c = number of lattice points on cell corners (shared by 8 cells)
- N_e = number of lattice points on cell edges (shared by 4 cells)

i = interior
f = face
c = corner
e = edge





Lattice Points- Review



$$N = 8 + \frac{0}{2} + \frac{8}{8} = 9 \text{ lattice points/unit cell}$$

Importance of the Number of Lattice Points

The number of lattice points tells you the number of atoms that are required to define your basis.

If $N = 4$, then four lattice points must be defined

Then, all you need to know is what types of atoms lie on each point.

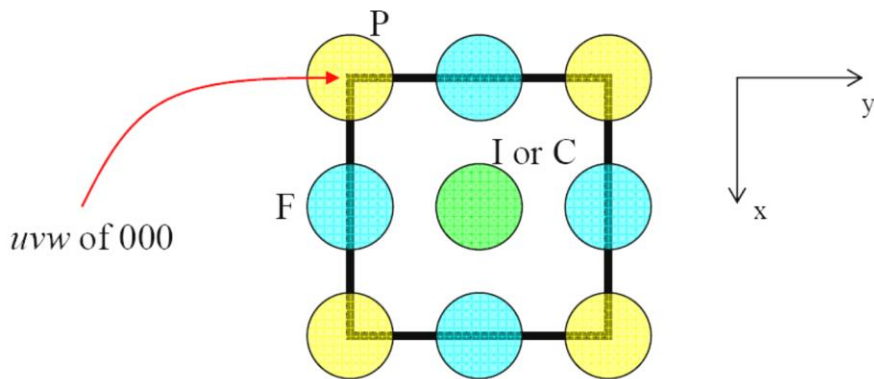
Arrangement of Lattice Points

ARRANGEMENT OF LATTICE POINTS

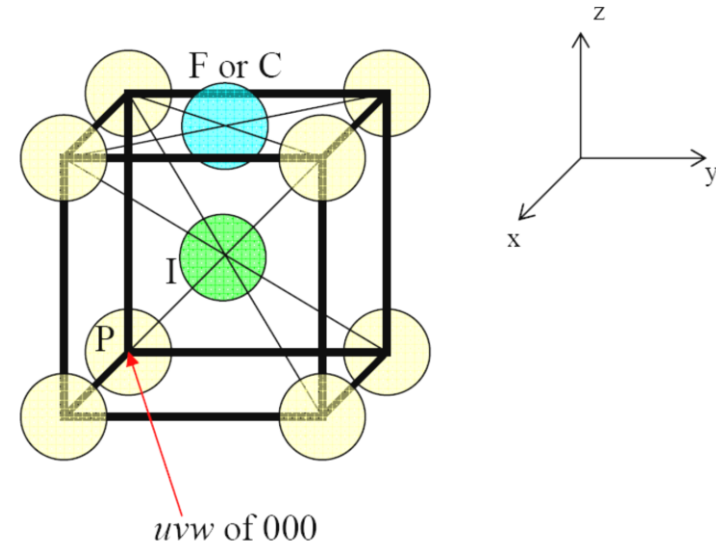
Each unit cell has a lattice point located at the corner (uvw of 000). This defines a primitive lattice (P)

Unit cells may also have them at the center of certain faces (F or C) or at the center (I) of the unit cell.

2-D



3-D





Arrangement of Lattice Points (continued)

Lattice points are categorized based on three possible centering operations (base, face, and body) + primitive (simple) arrangements

Name	Symbol	#Lattice Sites/Cell	Atom Locations
Primitive (simple)	P	1	000
Body-centered	I	2	000 $\frac{1}{2}\frac{1}{2}\frac{1}{2}$
Face-centered	F	4	000 $\frac{1}{2}\frac{1}{2}0$ $\frac{1}{2}0\frac{1}{2}$ $0\frac{1}{2}\frac{1}{2}$
Base-centered	C B A	2	000, $\frac{1}{2}\frac{1}{2}0$ 000, $\frac{1}{2}0\frac{1}{2}$ 000, $0\frac{1}{2}\frac{1}{2}$
Rhombohedral (this is a primitive cell)	R	1	000

•These are known as the *basis vectors*, which we will come back to.
•These are not *translation vectors (R)* since they have non-integer values.

The complexity of the system depends upon the symmetry requirements (is it lost or maintained?) by applying the symmetry operations (rotation, reflection, inversion and translation).



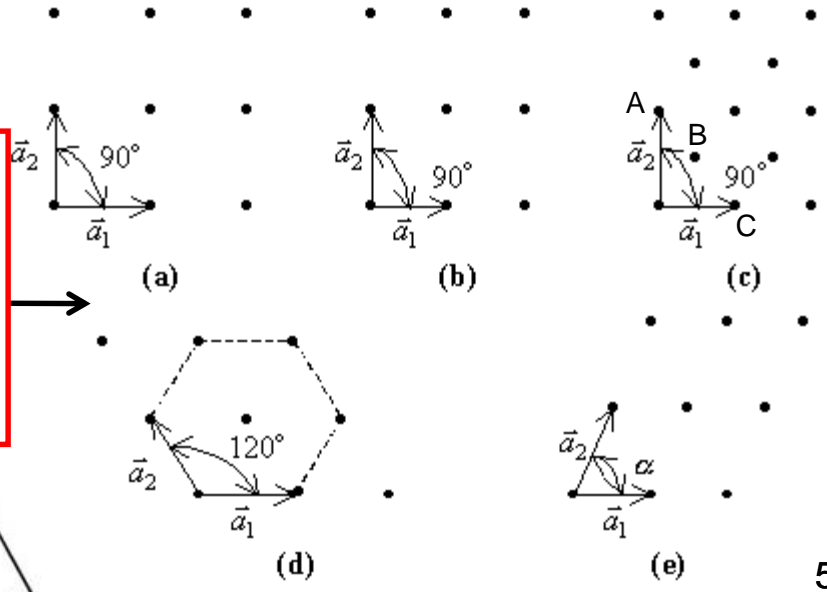
The Five 2-D Bravais Lattices

- From the previous definitions of the **four 2-D** and **seven 3-D** crystal systems, we know that there are **four** and **seven primitive unit cells** (with 1 lattice point/unit cell), respectively.
- We can then ask: can we add additional lattice points to the primitive lattices (or nets), in such a way that we still have a lattice (net) belonging to the same crystal system (with symmetry requirements)?
- First illustrate this for 2-D nets, where we know that the *surroundings of each lattice point must be identical*.
- We can come up with centered rectangular net in (c) where A, B and C points have identical surroundings.
- If we try to do same thing with other 2-D nets, we find that there are no new nets to be found...
- Two important ideas** are 1) it is always possible to define a primitive unit cell for every possible net and 2) if a non-primitive cell can be found that describes the symmetry of the net (lattice), then that cell should be used to describe the net (lattice). Since the surroundings of every lattice point must be identical, we can only add new lattice points at centered positions.

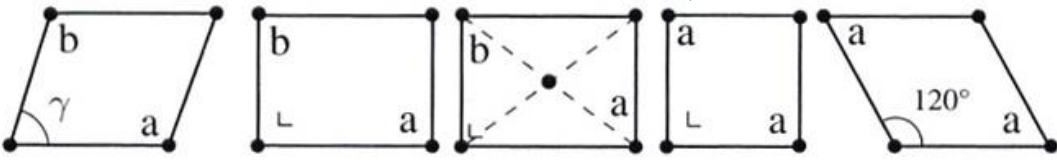
The 5 Bravais lattices of 2-D crystals: (a) square, (b) rectangular, (c) centered rectangular, (d) hexagonal and (e) oblique:

Name	Number of Bravais lattices	Conditions
Square	1	$a_1 = a_2, \alpha = 90^\circ$
Rectangular	2	$a_1 \neq a_2, \alpha = 90^\circ$
Hexagonal	1	$a_1 = a_2, \alpha = 120^\circ$
Oblique	1	$a_1 \neq a_2, \alpha \neq 120^\circ, \alpha \neq 90^\circ$

These are the only 5 possible 2-D Bravais lattices (4 primitive + 1 non-primitive)

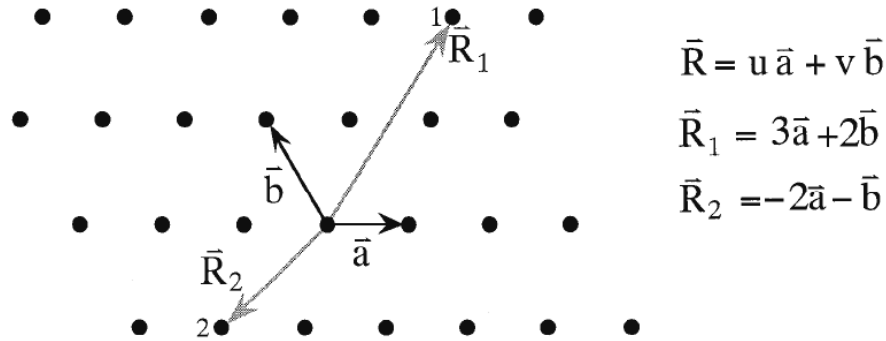


p. 72 in DeGraef



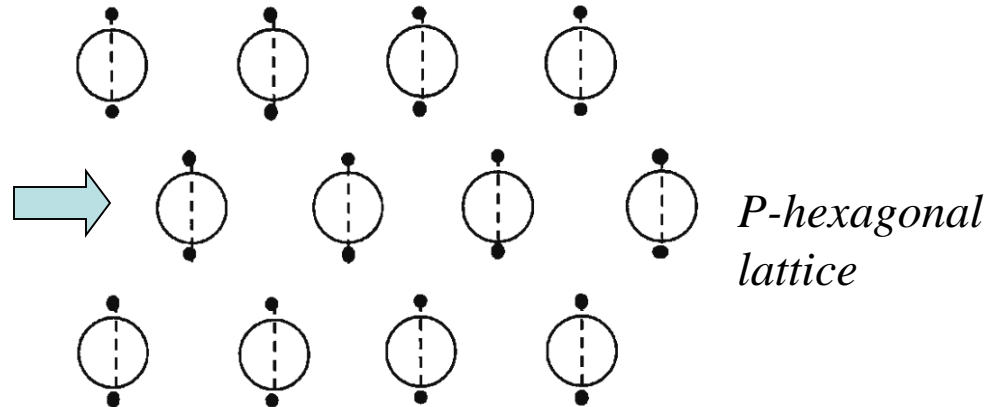
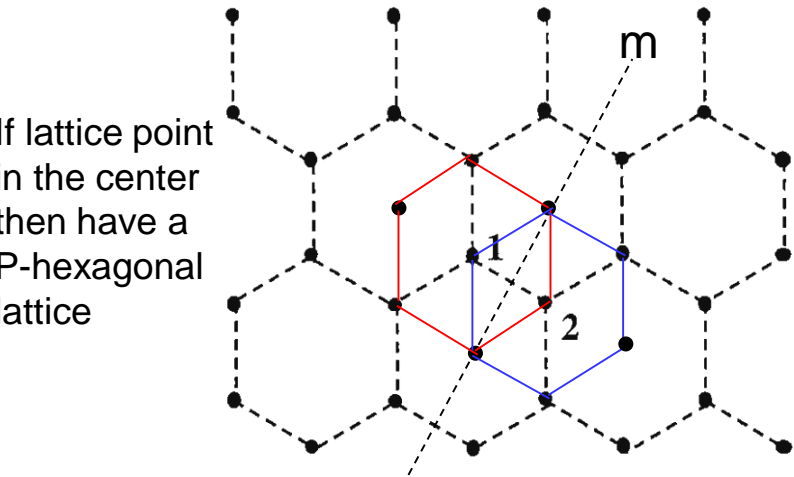
Bravais Lattice or Not?

This is a 2-D Bravais Lattice:



This is not a 2-D Bravais Lattice (when there is no lattice point in center of cell):

This is a 2-D Bravais Lattice:



If lattice point in the center then have a P-hexagonal lattice

From point 1 to 2: environment changes by reflection (mirror plane, m , half way in between), if you tie vertical pairs of points together then you have 2-D Bravais lattice with 6 identical neighbors.

The Fourteen 3-D Bravais Lattices

• We can repeat this procedure in 3-D, where there are 3 possible ways to add lattice points at the center between existing lattice points.

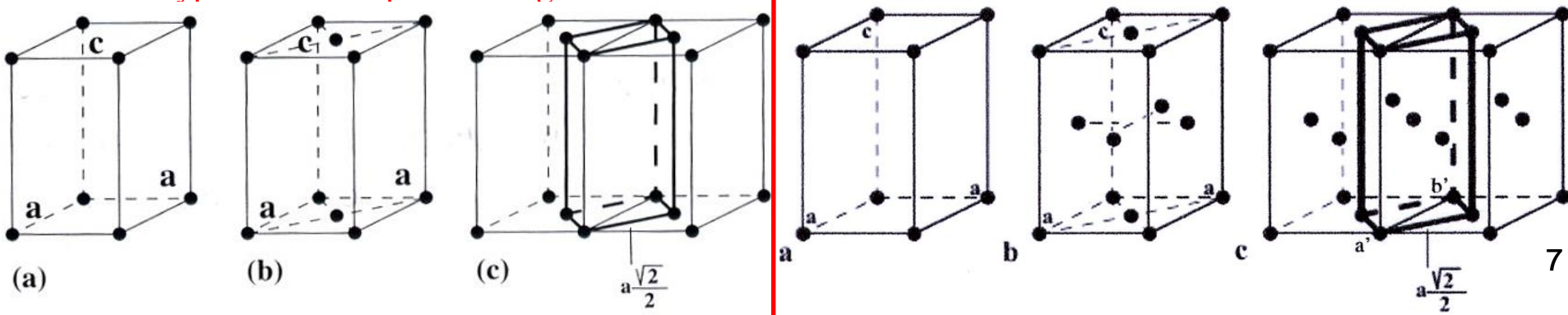
1. **Body centering**: we add a lattice site in the center of the unit cell at $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. For every site T there is an additional site $T + [(a+b+c)/2]$. The vector $I = [(a+b+c)/2]$ is body centering vector, note this is not a translation vector of lattice since its components are non-integers. The symbol for a body centered lattice is **I**.

2. **Face centering**: we add a lattice site to the center of all faces of the unit cell at $(\frac{1}{2}, \frac{1}{2}, 0)$, $(\frac{1}{2}, 0, \frac{1}{2})$, $(0, \frac{1}{2}, \frac{1}{2})$. For every site T , there are then 3 additional sites $T + [(a+b)/2]$, $T + [(a+c)/2]$, and $T + [(b+c)/2]$. The vectors $C = [(a+b)/2]$, $B = [(a+c)/2]$, $A = [(b+c)/2]$ are the face centering vectors. The symbol for a face centered lattice is **F**, where $\mathbf{F} = \mathbf{A} + \mathbf{B} + \mathbf{C}$.

3. **Base centering**: we add a lattice site to the center of only one face of the unit cell at $(\frac{1}{2}, \frac{1}{2}, 0)$ or $(\frac{1}{2}, 0, \frac{1}{2})$ or $(0, \frac{1}{2}, \frac{1}{2})$. The base centering vectors are identical to the face centering vectors, except that only one of them is present. If the plane formed by the basis vectors a and b is centered then the lattice is known as **C**-centered, if a and c is centered known as **B**-centered lattice and b and c is centered known as **A**-centered.

• We can now apply these 5 forms of centering (I,F,A,B,C) to all 7 primitive unit cell $\rightarrow 5 \times 7 = 35$ possibilities.

• In several cases we do generate a new lattice, in other cases we can redefine the unit cell and reduce the cell to another type. For example in tetragonal unit cells we only have P-tetragonal and I-tetragonal:





The Fourteen 3-D Bravais Lattices (continued)

•Repeating this exercise for all types of lattice centering, we end up with **7** additional lattice types that cannot be reduced to primitive ones of the same crystal system: **Cm, Co, Io, Fo, It, Ic, Fc.**

Add lattice points to crystal systems



14 BRAVAIS LATTICES

Represent the only ways to arrange points periodically in space while preserving lattice point surroundings, symmetry and uniqueness.

230 SPACE GROUPS (crystal structures)
32 CRYSTAL CLASSES
14 BRAVAIS LATTICES
7 CRYSTAL SYSTEMS (shapes)

This means that there are 7 types/shapes of crystals in 3-D from which we derive 14 types of lattices.

Bravais (1848) showed that there are 14 possible lattice point-crystal system combinations

Crystal Systems and Bravais Lattices

System	Axial lengths and angles	Bravais Lattice	Lattice Symbol
Cubic	$a = b = c; \alpha = \beta = \gamma = 90^\circ$	Simple	P
		Body-centered	I
		Face-centered	F
Tetragonal	$a = b \neq c; \alpha = \beta = \gamma = 90^\circ$	Simple	P
		Body-centered	I
Orthorhombic	$a \neq b \neq c; \alpha = \beta = \gamma = 90^\circ$	Simple	P
		Body-centered	I
		Base-centered	C
		Face-centered	F
Rhombohedral (trigonal)	$a = b = c; \alpha = \beta = \gamma \neq 90^\circ$	Simple	R
Hexagonal	$a = b \neq c; \alpha = \beta = 90^\circ; \gamma = 120^\circ$	Simple	P
Monoclinic	$a \neq b \neq c; \alpha = \gamma = 90^\circ \neq \beta$	Simple	P
		Base-centered	C
Triclinic	$a \neq b \neq c; \alpha \neq \beta \neq \gamma \neq 90^\circ$	Simple	P

“know these”

Only 14 based on 7 crystal systems + symmetry requirements!

•Reducing from 35 to 14 Bravais lattices means either the unit cell is not unique (choose one that is easier to work with) and/or symmetry of the crystal system is lost.

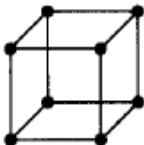
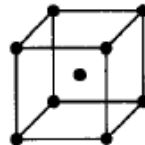
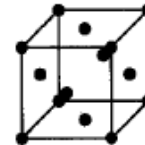
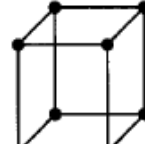
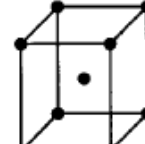
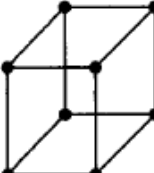
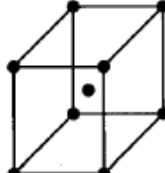
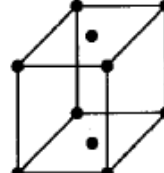
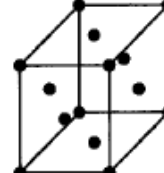
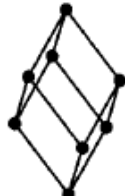
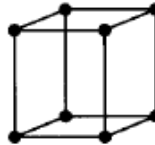
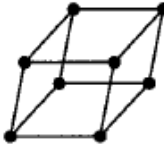
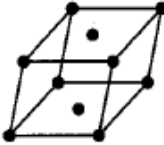

The Fourteen 3-D Bravais Lattices (continued)

These are the only 14 possible 3-D Bravais lattices

“know these”

14 Bravais Lattices

Table 3.2 *The Fourteen Crystal (Bravais) Lattices*

				
Simple cubic	Body-centered cubic (bcc)	Face-centered cubic fcc)	Simple tetragonal	Body-centered tetragonal
				
Simple orthorhombic	Body-centered orthorhombic	Base-centered orthorhombic	Face-centered orthorhombic	Rhomboidal
				
Hexagonal	Simple monoclinic	Base-centered monoclinic	Triclinic	

The Bravais lattices also represent the highest possible symmetry for the corresponding crystal systems.

Cubic Bravais Lattices

- This is a Bravais lattice because the 6-fold coordination of each lattice point is identical.

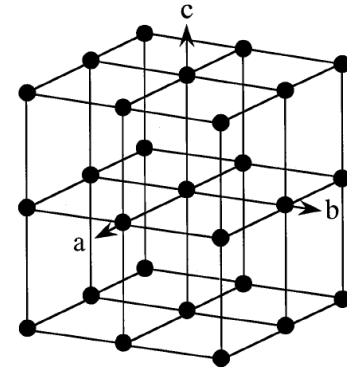
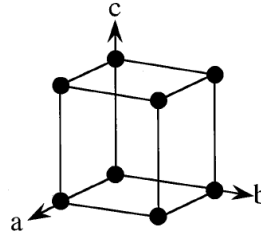
Remember crystal structure = lattice + basis (monoatomic in this case), and unit cell is the smallest portion of the lattice that contains both basis and the symmetry elements of the lattice.

- This is a Bravais lattice because the 8-fold coordination of each lattice point is identical.

- Notice that point 1 ($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$) at cube center and point 2 (0,0,0) at cube vertices have an identical 8-fold environment.

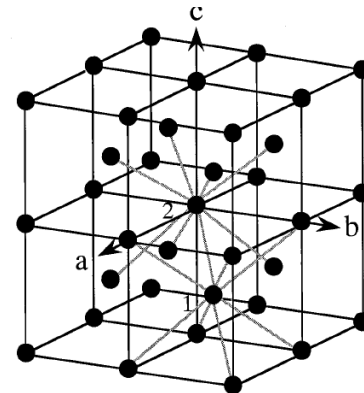
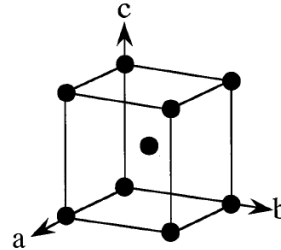
- This is a Bravais lattice because the 12-fold coordination of each lattice point is identical.

The *P*-cubic lattice



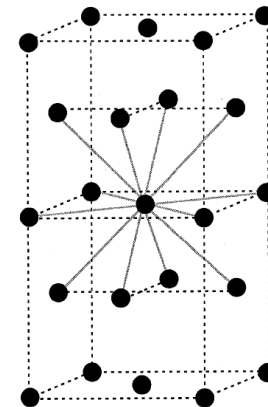
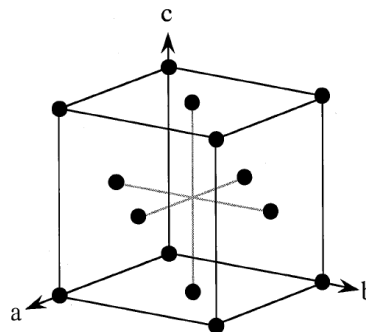
The extended *P*-cubic lattice

The *I*-cubic lattice



The extended *I*-cubic lattice

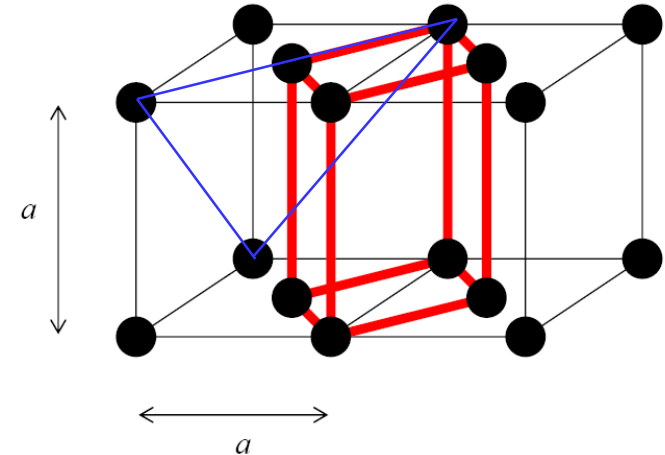
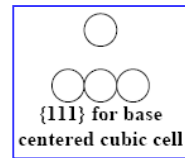
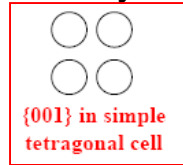
The *F*-cubic lattice



The extended *F*-cubic lattice

Cubic Bravais Lattices (continued)

- Why is there no base centered (A, B, or C)-cubic lattice?
- For example, no C-cubic lattice because a) it's simplified to *P*-tetragonal lattice (in red):
- Also note that b) the 3-fold symmetry (three 120° rotations) along the {111} is lost → variant (in blue):
- However, if you look down the {001} of *P*-tetragonal cell (in red) the 4-fold symmetry (four 90° rotations) is present:



Note that the nomenclature used for lattices is chosen to avoid confusion with crystal structures:

- In cubic systems: **SC**, **FCC**, and **BCC** are used to describe crystal structures, or more specifically the crystal structures created when an elemental, monoatomic basis is added to each site of the *P*, *F*, or *I*-cubic lattices, respectively.

- For example, tungsten atoms added to *I*-cubic lattice = **BCC** crystal structure
- Also, both rocksalt (e.g. NaCl) and sphalerite/zincblende (e.g. ZnS) have *F*-cubic lattices. However, we do not call these **FCC** crystal structures, since atoms in *FCC structure have 12 nearest neighbors* while atoms in *rocksalt structure have 6 nearest neighbors* and *4 in zincblende structure*.

- Thus we call them rocksalt and zincblende crystal structures or use Strukturbericht notation.

Tetragonal Bravais Lattices

• P and I tetragonal lattices are created when axial strain is put on their respective cubic lattices.

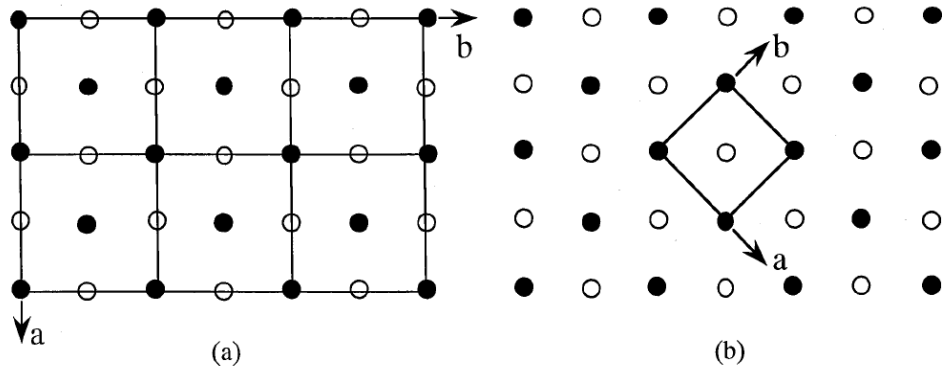
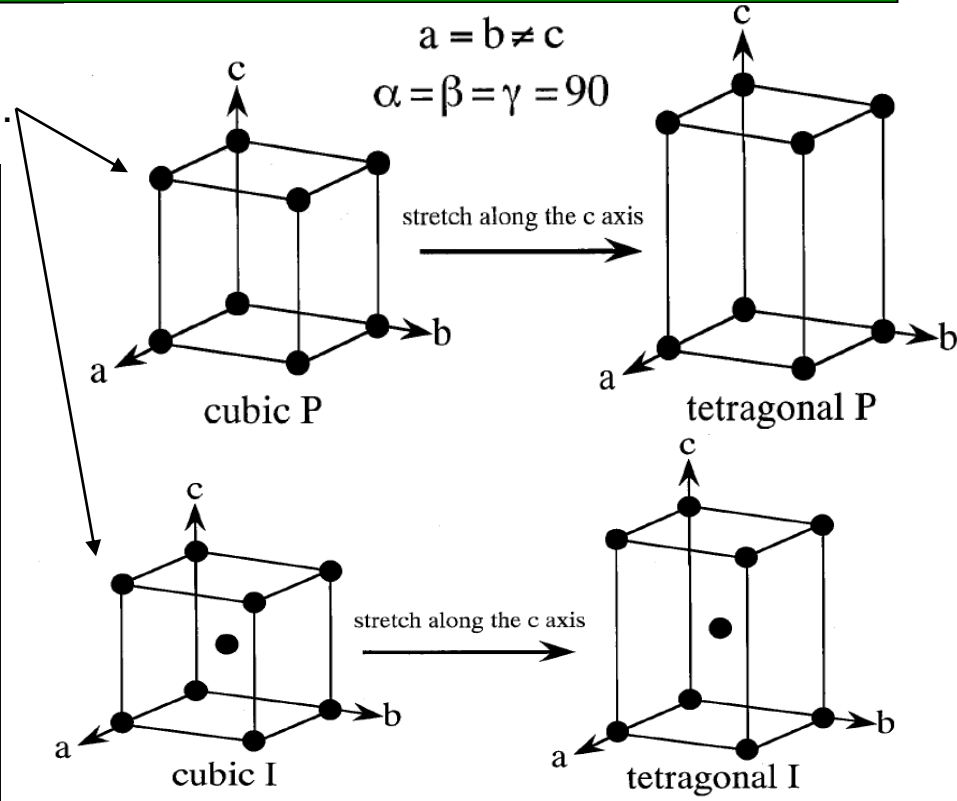
• Why not F-cubic lattice to F-tetragonal lattice?

• Because the result is identical to the *I*-tetragonal lattice, like we saw before in 3-D.

• Consider projection looking down *c*-axis in (a).

• By drawing new lattice vectors *a* and *b* rotated 45° with respect to original vectors and shorter by a factor of $\sqrt{2}/2$, we can define a *I*-tetragonal lattice from the same points in (b).

• So only one unique lattice is created, the *I*-tetragonal lattice, when *F* and *I*-cubic are strained.

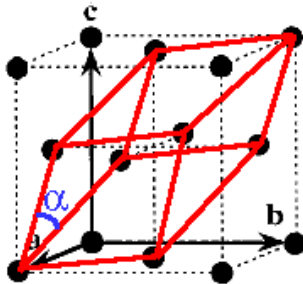


Dark points lie in plane of this 'slide' at $c=0$ and hollow points are at face centered positions at $c=1/2$.

*See DeGraef or Rohrer books for remaining Bravais lattices.

Other ways to define unit cell

- It is always possible to describe a lattice with a primitive unit cell.
- Thus, all 14 Bravais lattices can be described by primitive cells, even when they are centered (non-primitive).
- For example, consider the **non-primitive Fc (FCC) lattice**:
 - By selecting shorter vectors a_1 , a_2 , and a_3 , we can define a **primitive rhombohedral lattice** with angle $\alpha=60^\circ$.
- We can draw this:



- There is also the [Wigner-Seitz \(WS\) cell](#), which you will see in the *Electrical Properties of Materials* class or textbook, to describe the first Brillouin zone of the reciprocal lattice.
- Brillouin zones are used in band theory to represent in reciprocal space the solutions of the wave equations for the propagation of phonons or electrons in solids.



Minimum Symmetry Requirements

•Based on the symmetry operations, the minimal requirements for the 7 crystal systems in 3-D are:

1. Triclinic, all cases not satisfying the requirements of any other system; thus there is no symmetry other than translational symmetry, or inversion ($\bar{1}$) or identity (1) in 3-D.
2. Monoclinic, requires either 1 two-fold axis of rotation (180°), or 1 mirror (m) plane, or 1 combined 2/m operation.
3. Orthorhombic, requires either 3 two-fold axes of rotation (180°), or 1 two fold axis of rotation (180°) and two mirror (m) planes, *or* combination of 3 total two-fold rotation(s) & mirror(s).
4. Tetragonal, requires 1 four-fold axis of rotation (90°).
5. Rhombohedral (trigonal), requires 1 three-fold axis of rotation (120°) along one body diagonal.
6. Hexagonal, requires 1 six-fold axis of rotation (60°).
7. Cubic, requires 4 three-fold axes of rotation (120°) along all 4 body diagonals.

“know these”