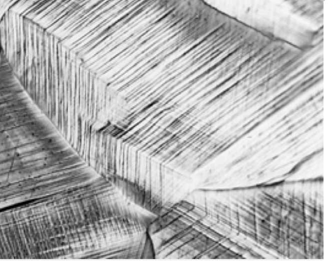
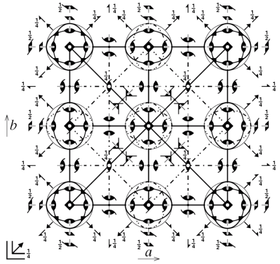
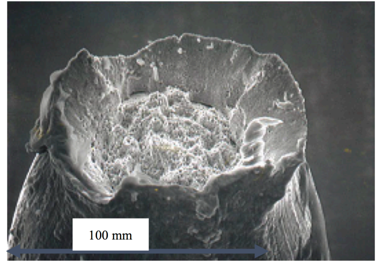
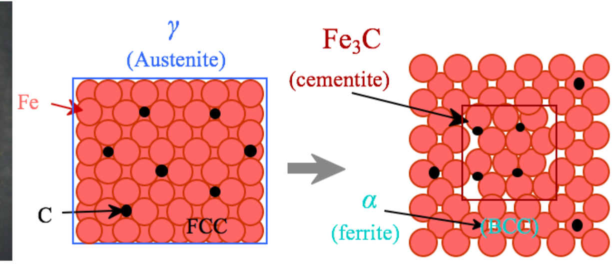






MEAM/MSE 507
Fundamentals of Materials

Prof. Jordan R. Raney

Week 4, Lecture 2: Bravais lattices

Asynchronous

2D symmetry operations

Symmetry operations involve transformation of coordinates:

1. Translation

$$(x,\ y) \xrightarrow{\vec{T}} (x+a,\ y+b) \xrightarrow{\vec{T}} (x+2a,\ y+2b)$$

2. Mirror / reflection

   Need to define a "mirror axis" (in 2D) or "mirror plane" (in 3D)

   E.g., for a mirror axis parallel with the y-axis in 2D:

$$(x,\ y) \xrightarrow{M} (-x,\ y) \xrightarrow{M} (x,\ y)$$

M changes the sense of *one* coordinate

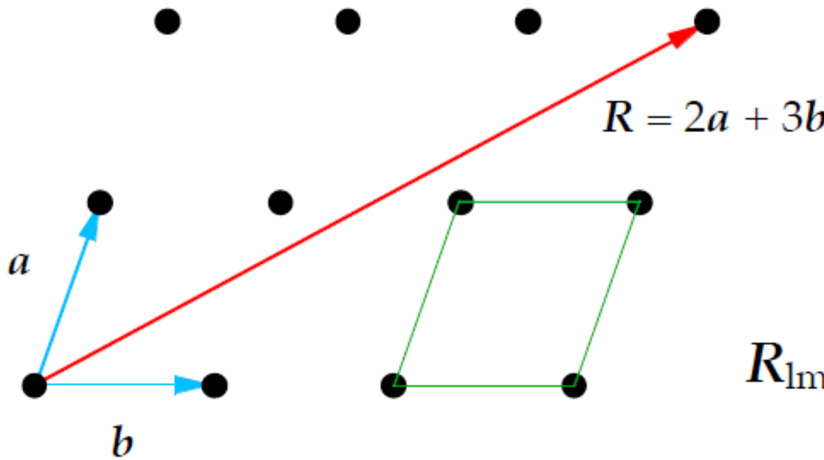
3. Rotation

   Need to define a point (in 2D) or axis (in 3D) around which rotation occurs. E.g., $\boldsymbol{A}_\pi$ rotates everything by π radians around point *A*.

Rotation can change the sense of *two* coordinates

The space lattice

- Every point in the space lattice is identical
- The translation vector tells how to get from any point to any other equivalent point

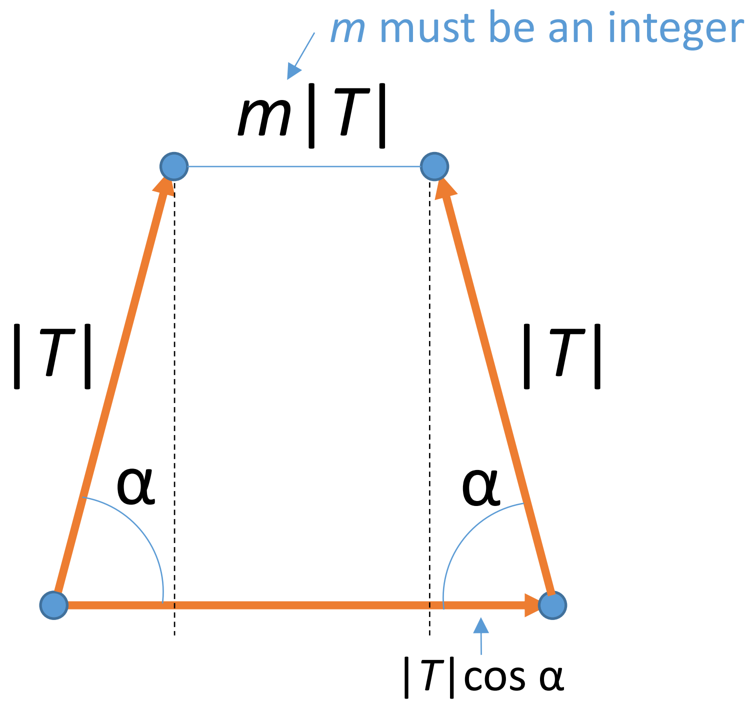


$$R_{lmn} = la + mb + nc$$

- a, b, c are lattice vectors; l, m, n are integers
- A good set of lattice vectors allows the translation vector to span from any point in the lattice to any other
- Unit cell is parallelepiped whose edges are a, b, c

What types of lattices are possible given the known symmetry operations?

Rotational symmetry and space-filling lattices



$$|T| - 2|T|\cos\alpha = m|T|$$

$$\Rightarrow 1 - 2\cos\alpha = m$$

$$\Rightarrow \cos\alpha = \frac{1-m}{2}$$

Rotational symmetry and space-filling lattices

Any m >= 4 does not have a valid value for α

m	$\frac{1-m}{2}$	α	n-fold axes
4	-3/2	Not possible	
3	-1	π (180°)	2-fold
2	-1/2	$2\pi/3$ (120°)	3-fold
1	0	$\pi/2$ (90°)	4-fold
0	1/2	$\pi/3$ (60°)	6-fold
-1	1	0	1-fold
-2	3/2	Not possible	

Any m <= -2 does not have a valid value for α

Only these rotational symmetries are allowed in a space-filling lattice!

Penn Engineering

Symmetry operations in 2D

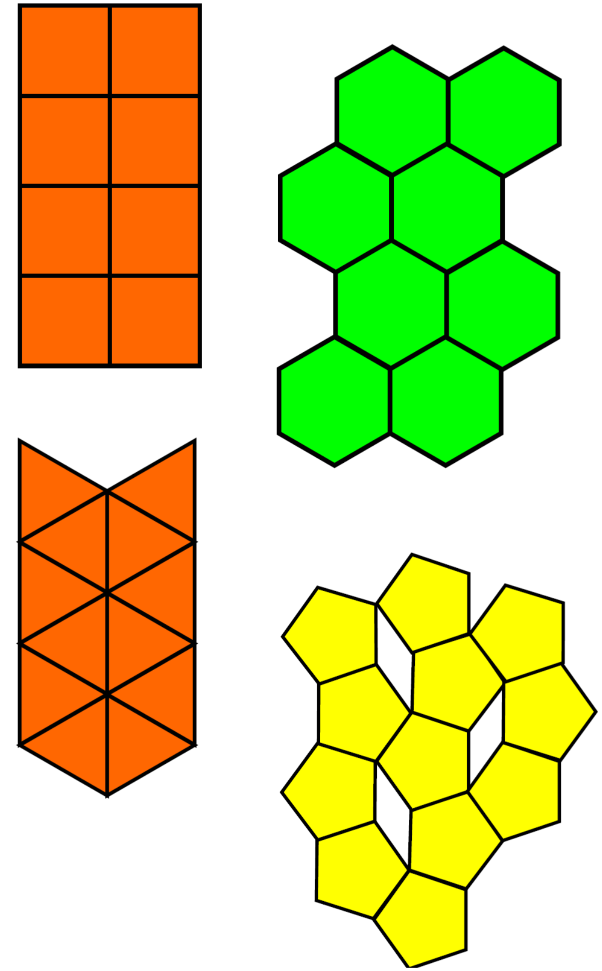
- Translation
- Reflection
- Rotation
  - *n*-fold rotation mean $2\pi/n$

2-fold (180˚ rotation)

3-fold (120˚ rotation)

4-fold (90˚ rotation)

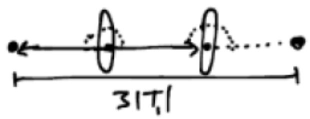
6-fold (60˚ rotation)



- *n* can also be 1 (trivial or identity)

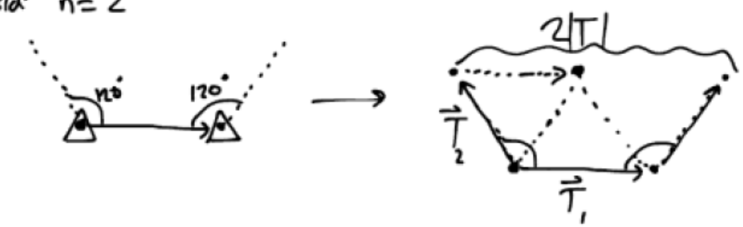
Building up a 2D lattice from **translation** and **rotation**

E.g., 2-fold: n=3



No effect on row above, so $\vec{T}_2$ can be very different

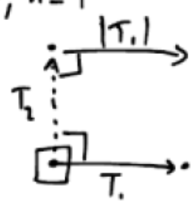
E.g., 3-fold: n=2



$|\vec{T}_1| = |\vec{T}_2|$

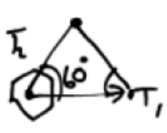
angle between $\vec{T}_1$, $\vec{T}_2$ = 120°

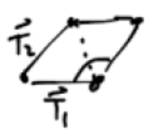
E.g., 4-fold, n=1



Need $|\vec{T}_1| = |\vec{T}_2|$ and angle 90°

E.g., 6-fold, n=0





$|\vec{T}_1| = |\vec{T}_2|$
Can describe angle as 120°

Same as 3-fold

Convention: use $\alpha \geq 90°$ rather than small angle option

Allowed 2D lattices (the 5 Bravais lattices)

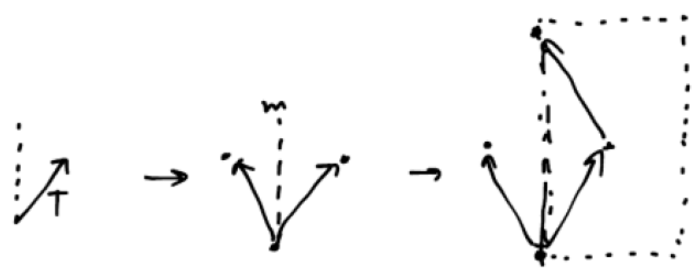
kinds of 2D lattices:

$\left.\begin{array}{l} \underline{\text{Oblique/Parallelogram}}: |\vec{T}_1| \neq |\vec{T}_2|, \text{ angle any, can accommodate } 1 \text{ or } ⬯ \\ \underline{\text{hexagonal}}: |\vec{T}_1| = |\vec{T}_2|, \text{ angle } 120^\circ, \text{ can accommodate } \triangle \text{ or } ⬡ \\ \underline{\text{square}}: |\vec{T}_1| = |\vec{T}_2|, \text{ angle } 90^\circ, \text{ can accommodate } \square \end{array}\right\}$ These come from translation + rotation

Other lattices? Yes, if we add reflection:

<u>Centered rectangular/rhombohedral</u>

$|\vec{T}_1| \neq |\vec{T}_2|$, but angle 90°, w/ 2 lattice points per cell



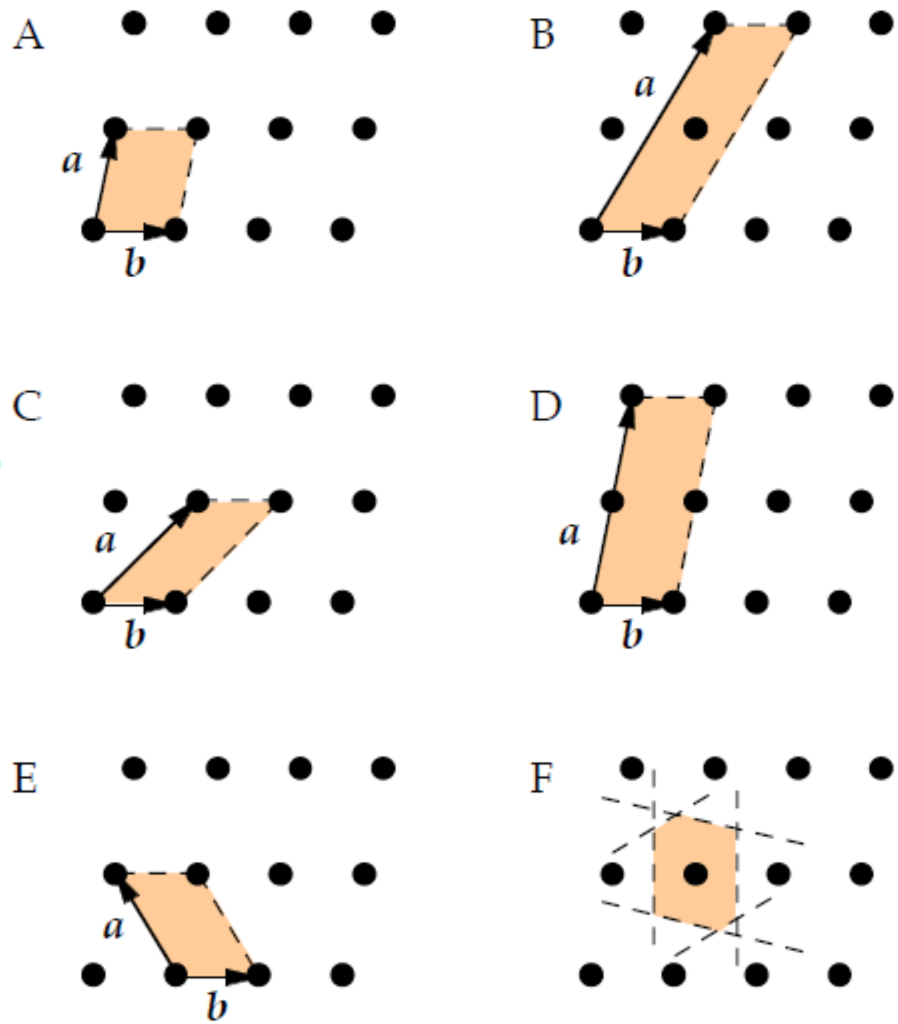
<u>primitive rectangular</u>

Same as above but without the center point

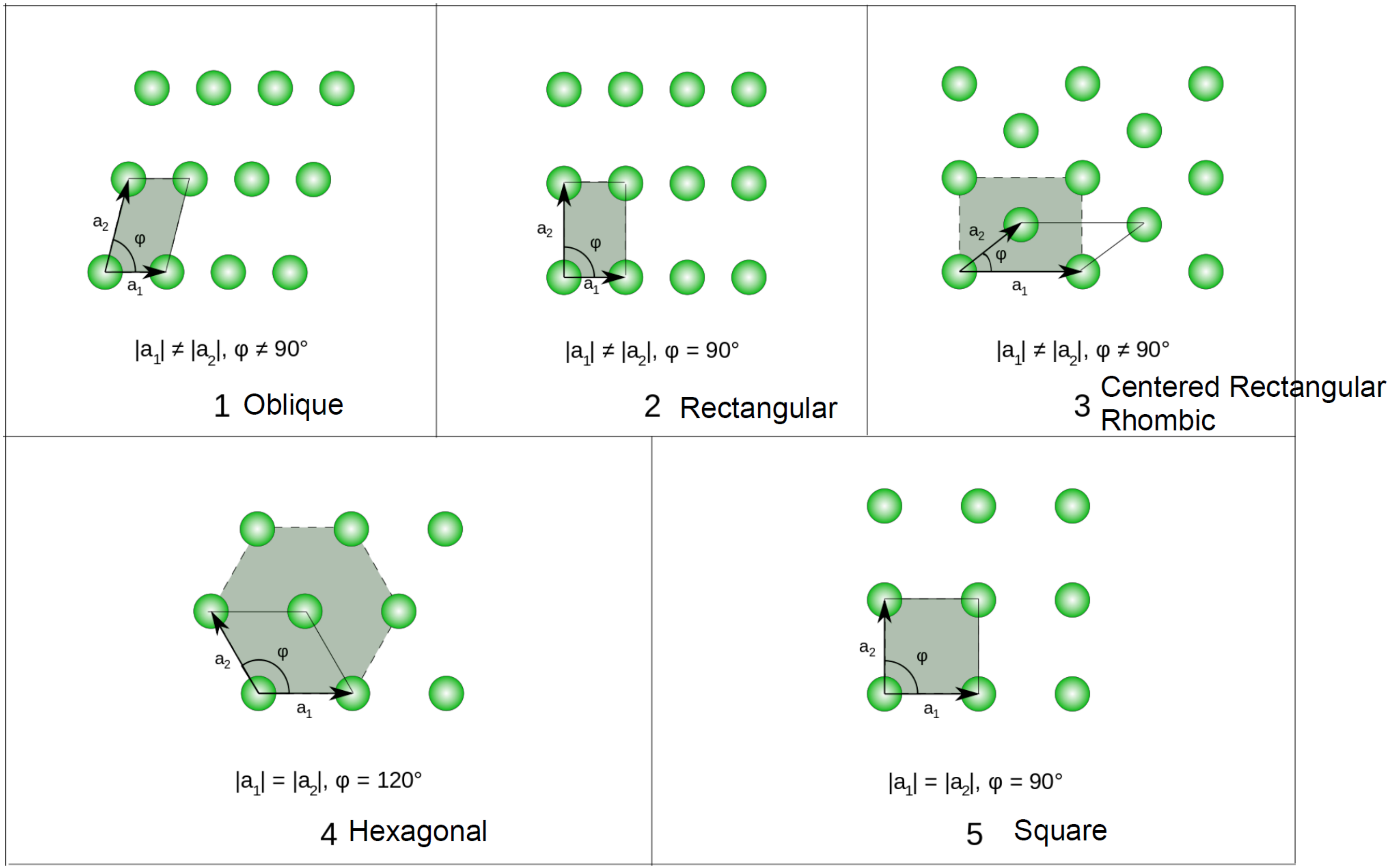
Unit cell

Primitive lattice vectors define a primitive unit cell

- That is, a cell that contains a single lattice point
- Which are primitive?
- Wigner-Seitz primitive cell puts the lattice point at the "center"



Bravais lattices in 2D

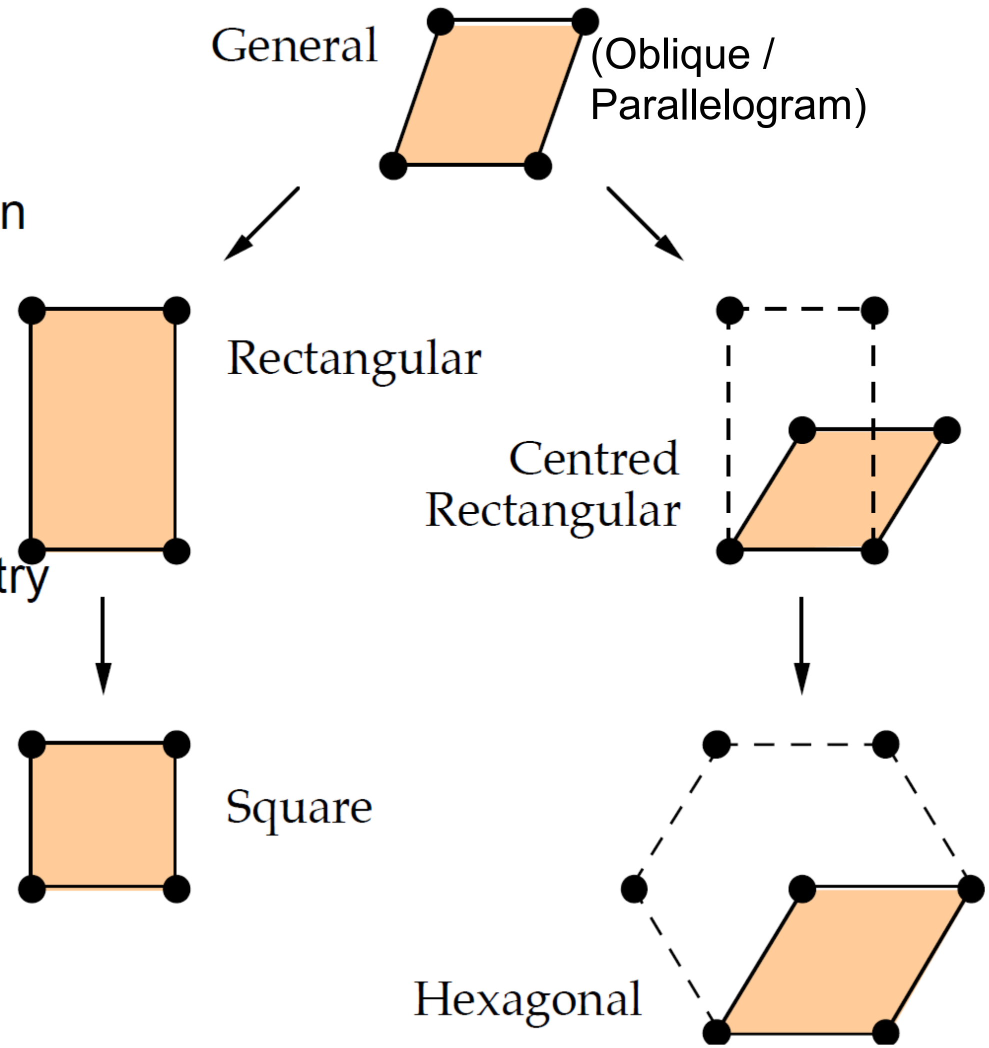


Bravais lattices in 2D

- Bravais lattice is an infinite array of discrete points generated by

$$\boldsymbol{R}_{lmn} = l\boldsymbol{a} + m\boldsymbol{b} + n\boldsymbol{c}$$

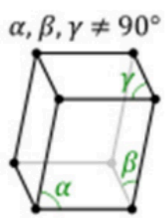
- Infinite number of space lattices can be formed by choosing $\boldsymbol{a}$, $\boldsymbol{b}$, $\boldsymbol{c}$ in 3d or $\boldsymbol{a}$, $\boldsymbol{b}$ in 2d
- From any R_{lmn} the lattice looks exactly the same
- Most lattices only have the symmetry n=1 or 2, but we can choose $\boldsymbol{a}$, $\boldsymbol{b}$, $\boldsymbol{c}$ to get other symmetries
- These symmetries imply restriction on $\boldsymbol{a}$, $\boldsymbol{b}$, $\boldsymbol{c}$
- Each set of restrictions → distinct lattice; a Bravais lattice is characterized by its symmetry operations



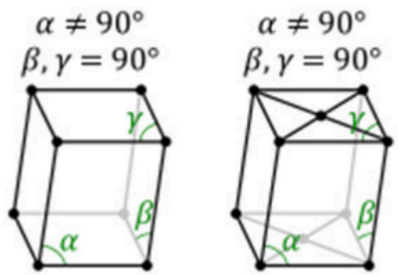
2d: 4 restrictions→ 5 lattices

Bravais lattices in 3D

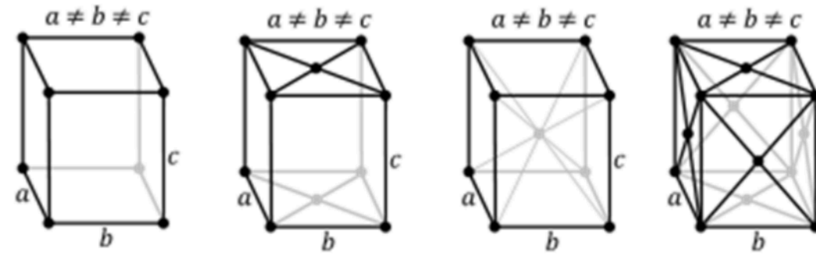
Triclinic



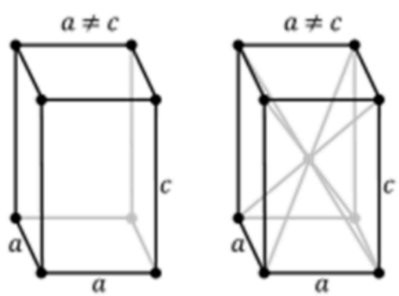
Monoclinic



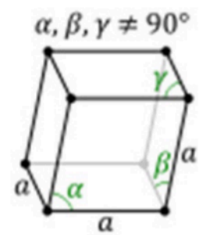
Orthorhombic



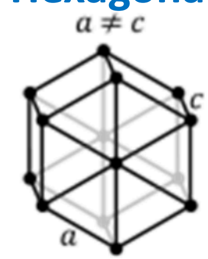
Tetragonal



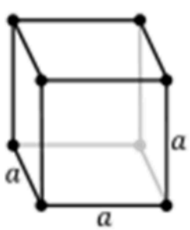
Trigonal/rhombohedral



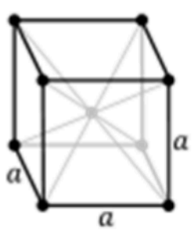
Hexagonal



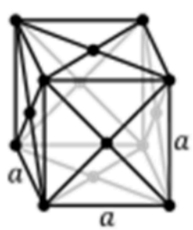
Cubic



Simple Cubic



Body Centered Cubic



Face Centered Cubic

- **14 Bravais lattices in 3D**
- **7 crystal systems**