Review the survey

We Start From the Beginning

- Warning: section 1.1 of the book is very DENSE and difficult to UNDERSTAND
- It is an attempt to condense several chapters of crystallography into a few pages.
- We will EXPAND upon this material in the next few lectures
- Other helpful ONLINE resources:
  - West, *Solid State Chemistry and its Applications*
  - Hammond, *The Basics of Crystallography and Diffraction*

A Comprehensive Mathematical Framework for Describing Crystals

- One way to describe crystals is to look at the packing of the atoms using spheres as spherical representations. This is good for building some intuition.
- However, it is not good for understanding ALL POSSIBLE CRYSTALS, you would be overwhelmed with trivia.
- What if you could come up with the minimum mathematical framework to describe all crystals?

Translational Symmetry in 2D

Goal

•Build intuition for lattices & unit cells in 2D
•See why only certain symmetries work in crystals

Learning Objectives

•Differentiate crystalline vs amorphous solids
•Define lattice, vectors, unit cell
•Identify shapes that tile space
•Recognize allowed rotation axes (2, 3, 4, 6-fold)
•See how lattice + motif → crystal (e.g. graphene)

Relationship to Text

•*Structures of Crystalline Materials*, Ch. 1 (pp. 1–12)
•1.1.1 Translational Symmetry (pp. 2–3)
•1.1.2 Rotational Symmetry (pp. 3–5)
•1.1.3 Crystal Systems (pp. 5–6)
•1.1.4 Bravais Lattices (pp. 6–8)

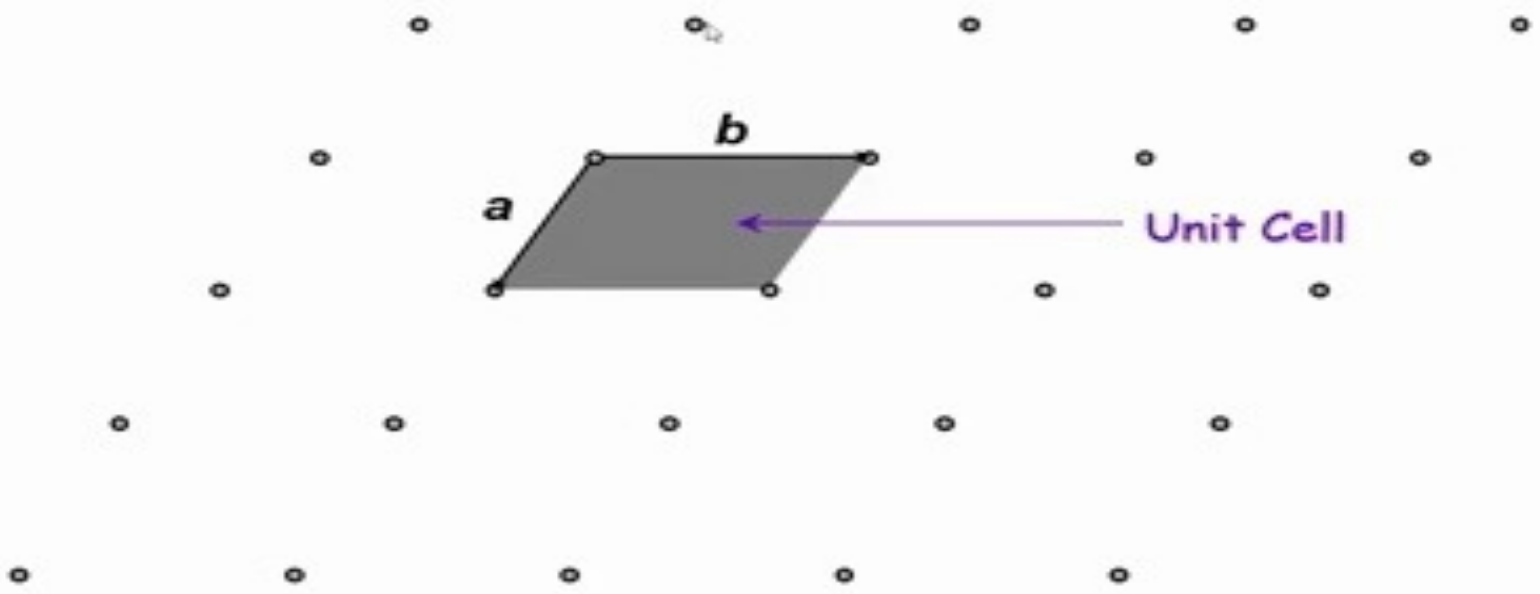
Crystalline vs. Amorphous Solids

Iron pyrite
(FeS_2)
a crystalline solid

Obsidian
(typically $KAlSi_3O_8$)
an amorphous solid

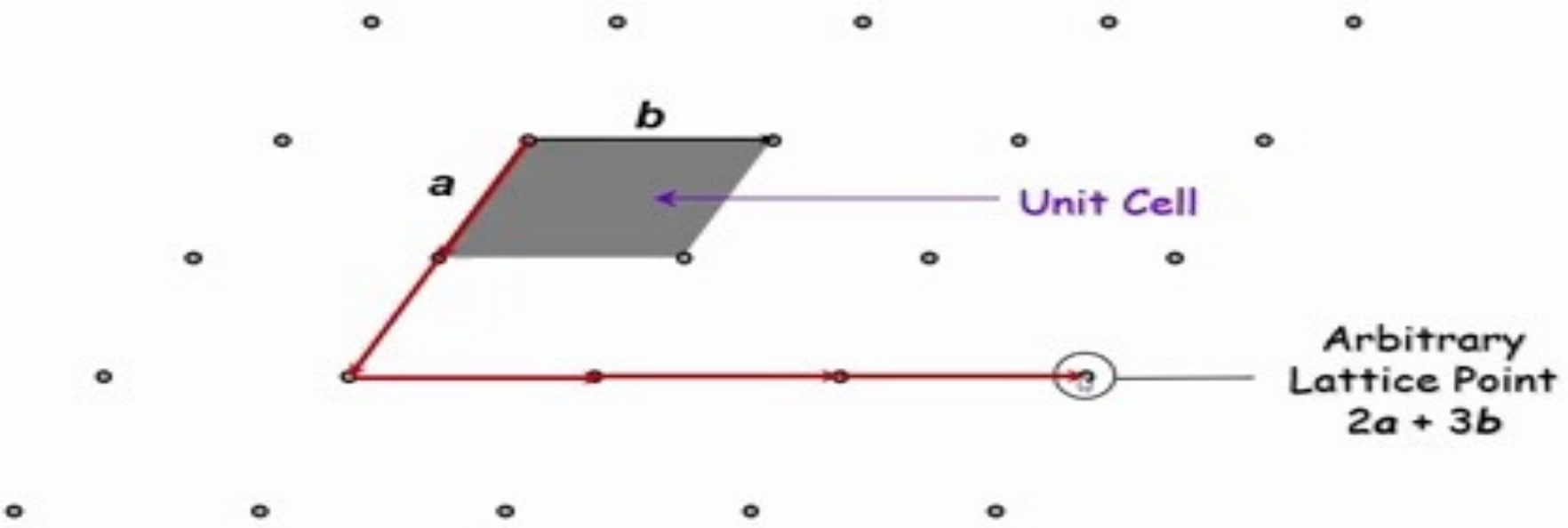
Crystalline solids possess translational symmetry, amorphous solids do not
(they are like frozen liquids)

Translational Symmetry (in 2D)



- ***a*** and ***b*** are the lattice vectors, every lattice point can be defined by adding these two vectors (in 2D)
- The unit cell is the **parallelogram** defined by the lattice vectors, all space can be filled by tiling unit cells.

Translational Symmetry (in 2D)

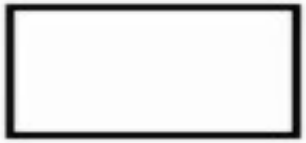


- ***a*** and ***b*** are the lattice vectors, every lattice point can be defined by adding these two vectors (in 2D)
- The unit cell is the **parallelogram** defined by the lattice vectors, all space can be filled by tiling unit cells.

Which shapes can we use to tile space

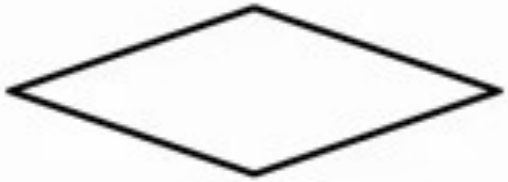
triangle

square

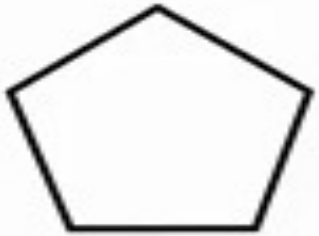


rectangle

parallelogram

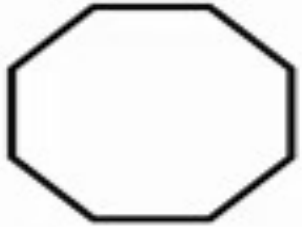


rhombus



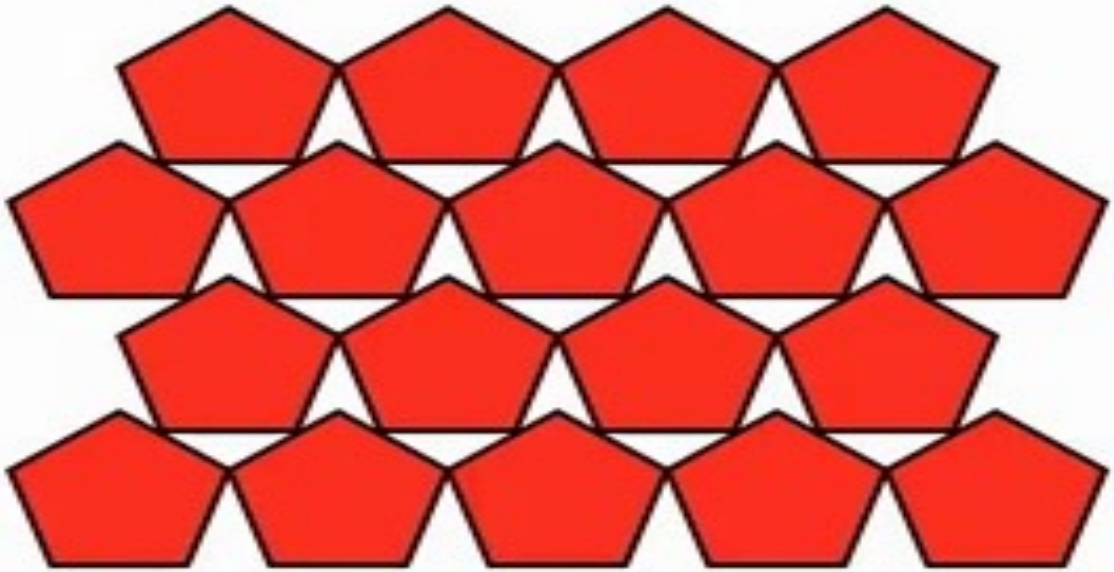
pentagon

hexagon



octagon

Not all shapes can tile space



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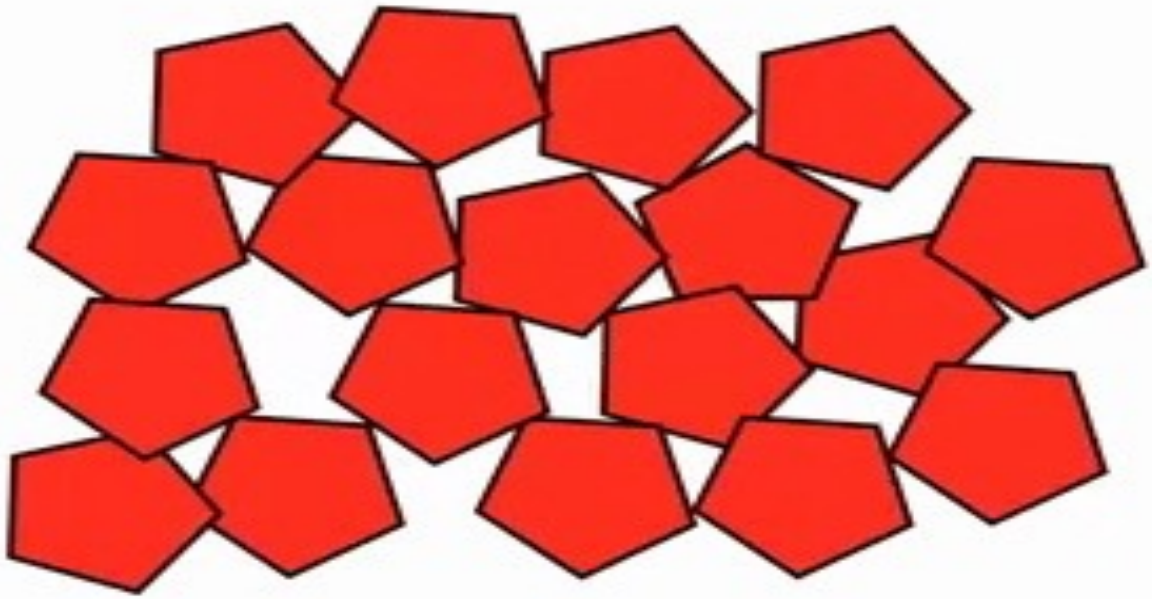

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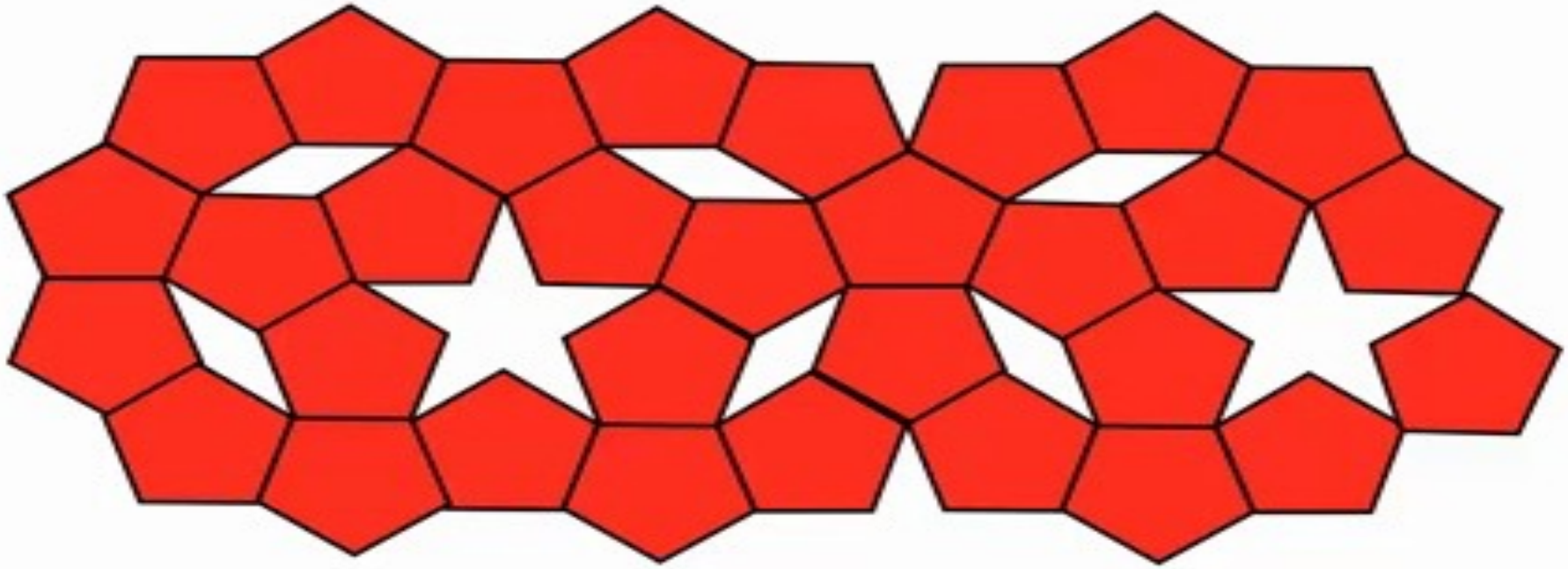
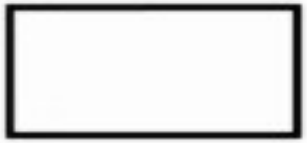


Only 2-fold, 3-fold, 4-fold and 6-fold axes can be realized in a crystal

Which shapes can we use to tile space

triangle

square



rectangle

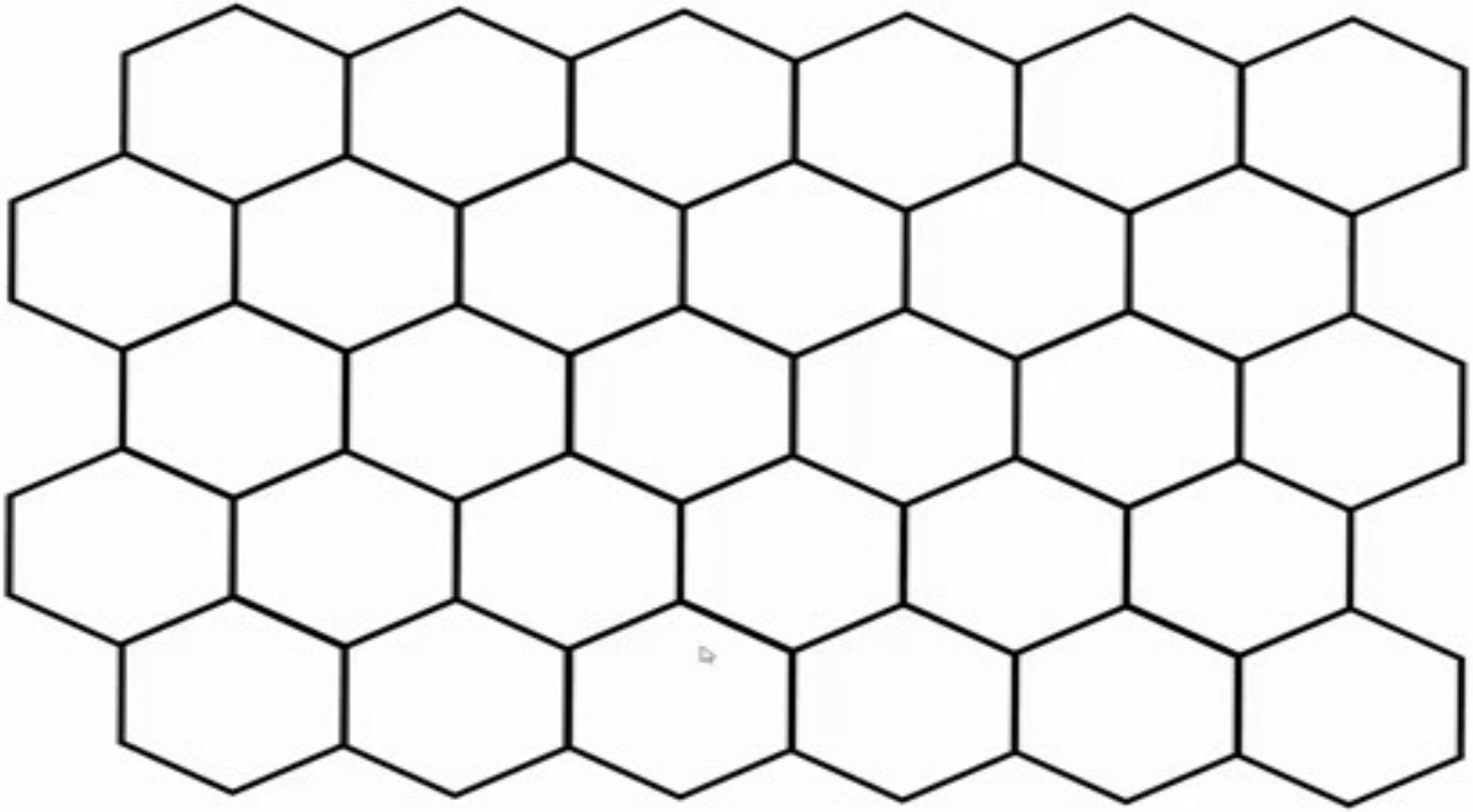
parallelogram

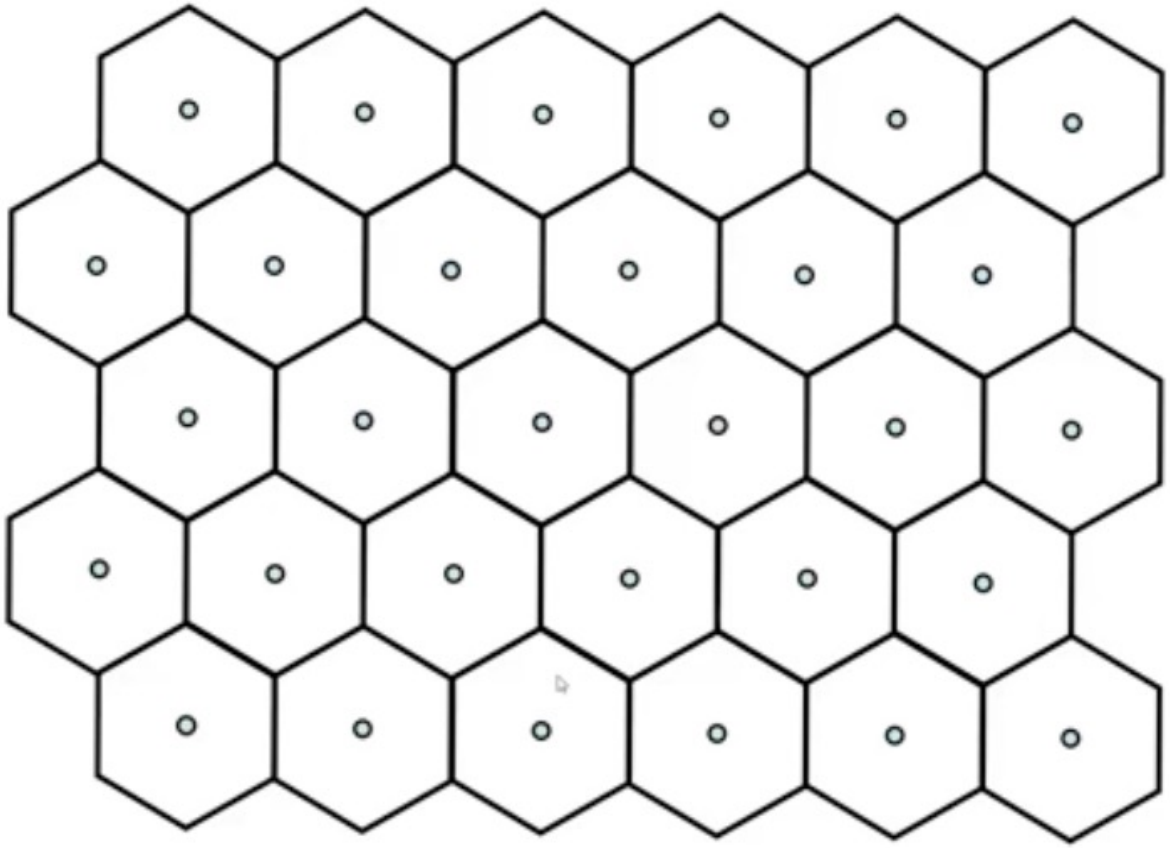
rhombus

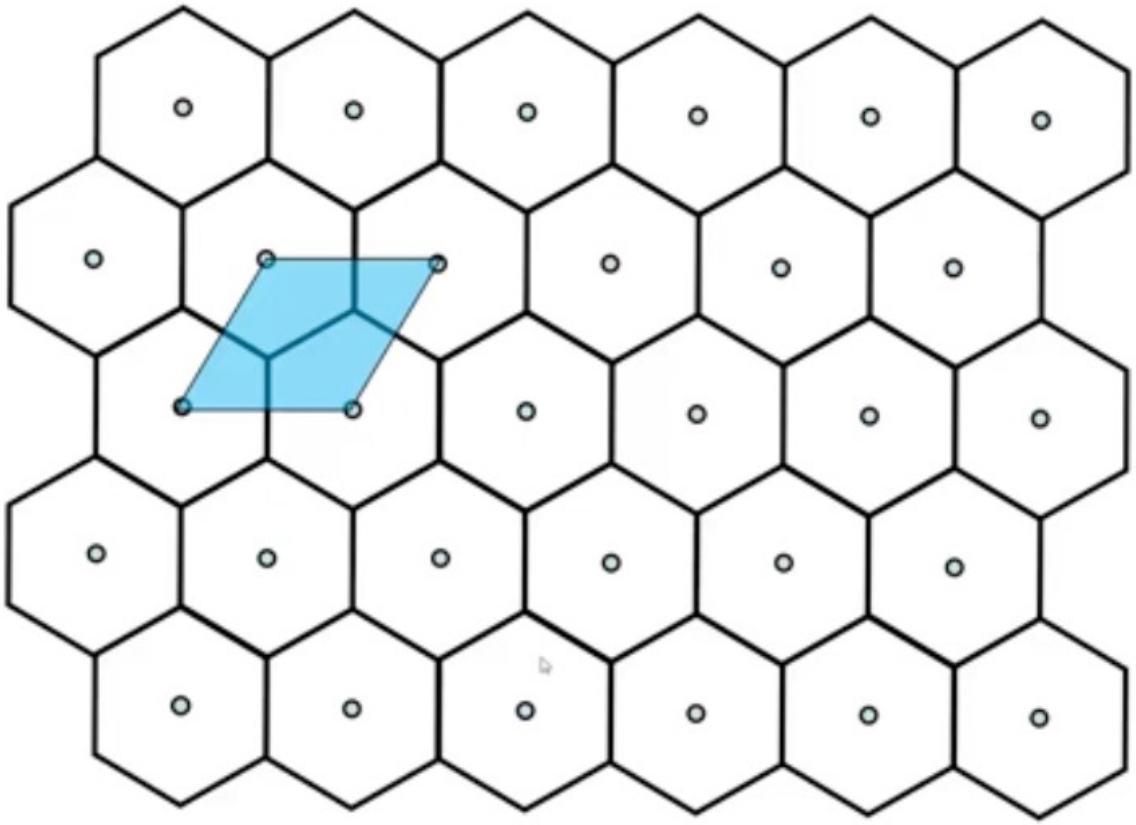
pentagon

hexagon

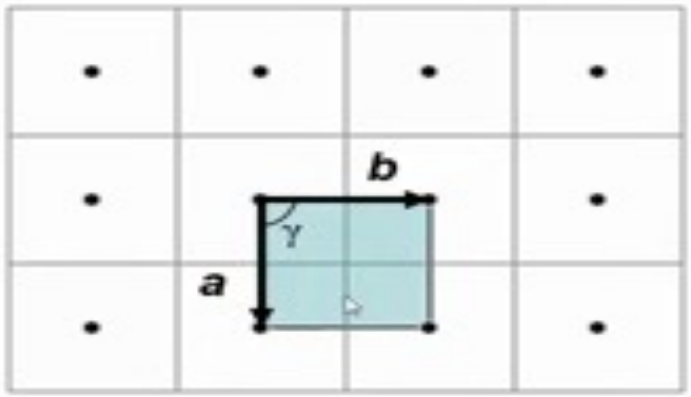
octagon



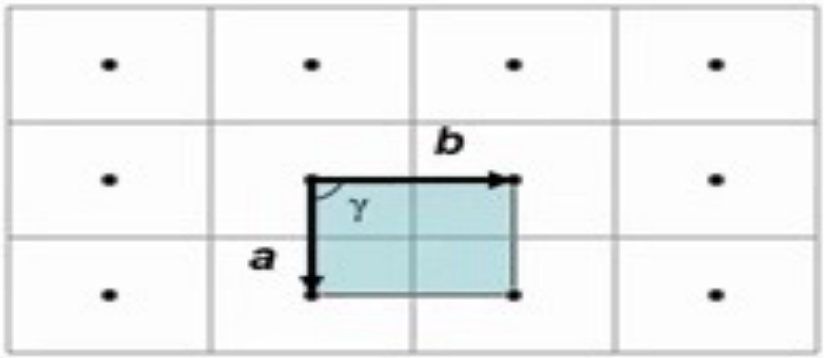




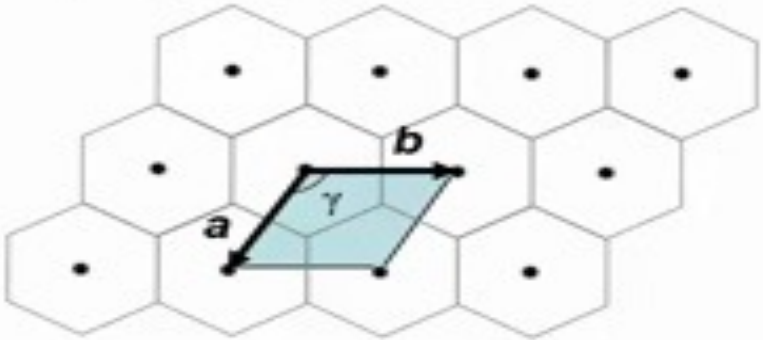
2D Crystal systems



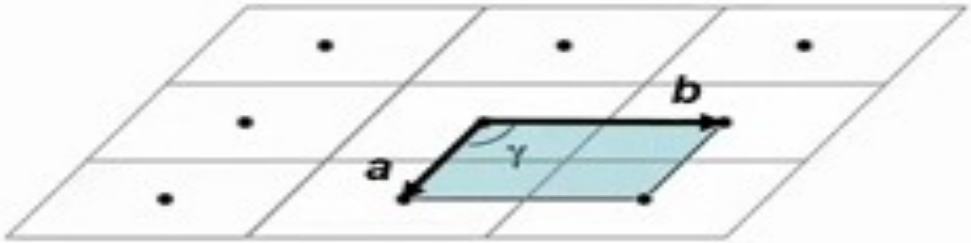
Square lattice ($a = b$, $\gamma = 90°$)
Req. Symmetry: 4-fold rotation axis



Rectangular lattice ($a \neq b$, $\gamma = 90°$)
Req. Symmetry: mirror or glide plane

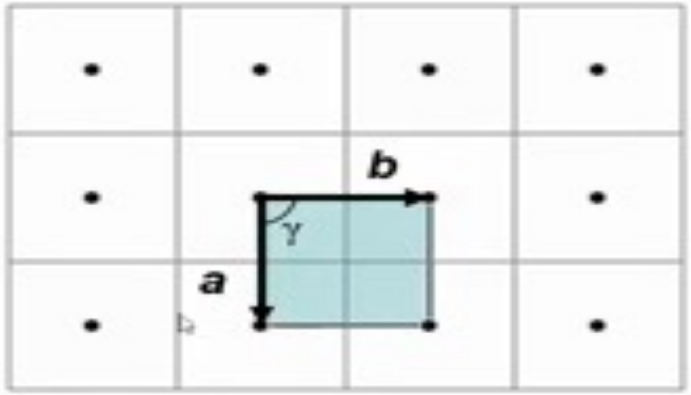


Hexagonal lattice ($a = b$, $\gamma = 120°$)
Req. Symmetry: 3- or 6-fold rotation axis



Oblique lattice ($a \neq b$, γ = arbitrary)
Req. Symmetry: None

2D Crystal systems



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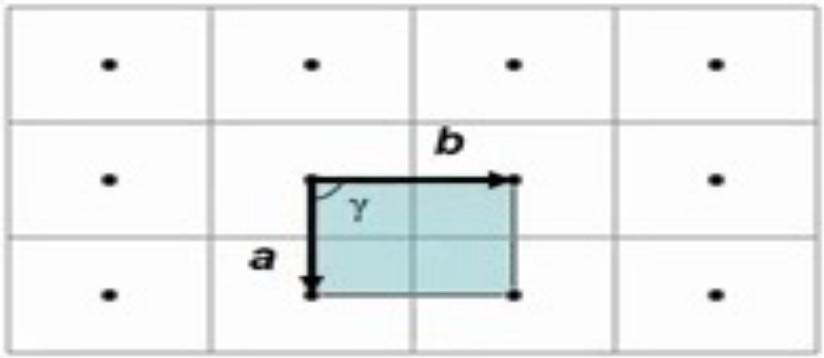

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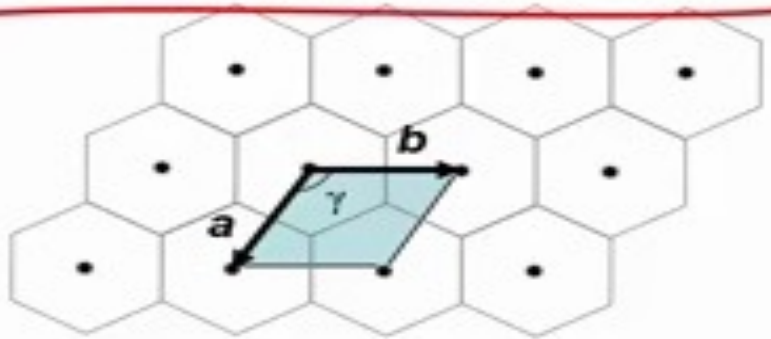

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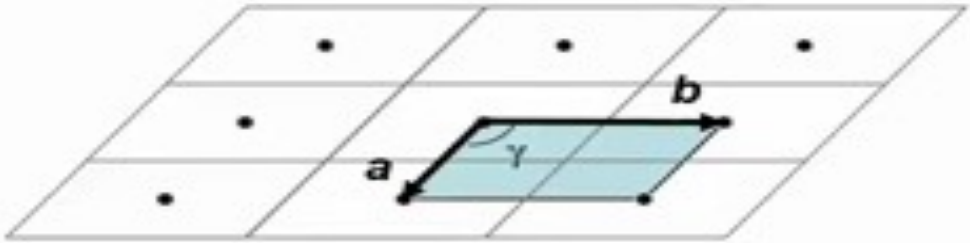

Oblique lattice ($a \neq b$, γ = arbitrary)
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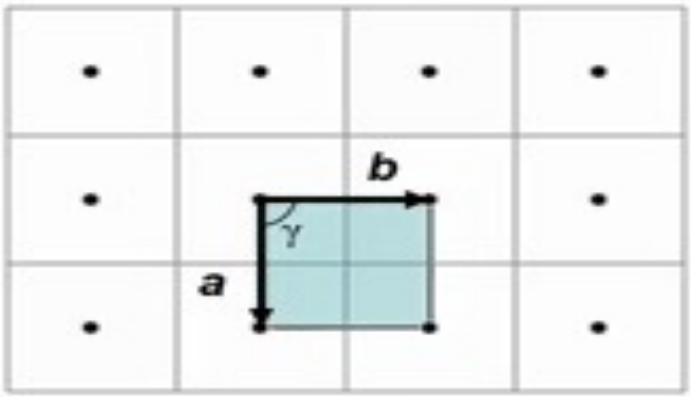
2D Crystal systems



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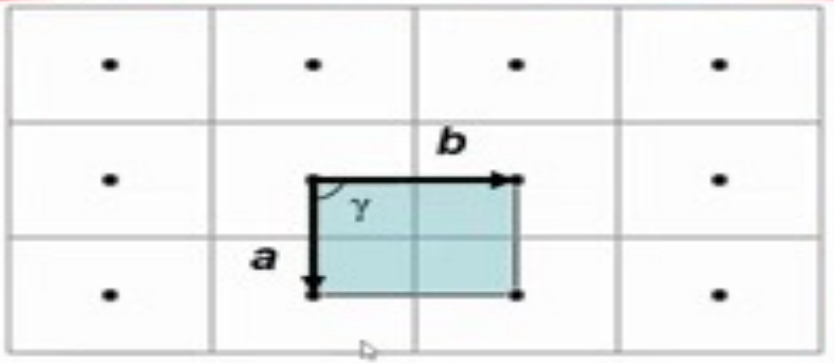

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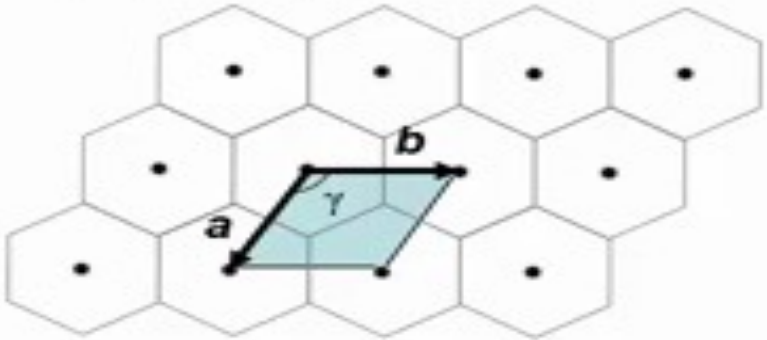

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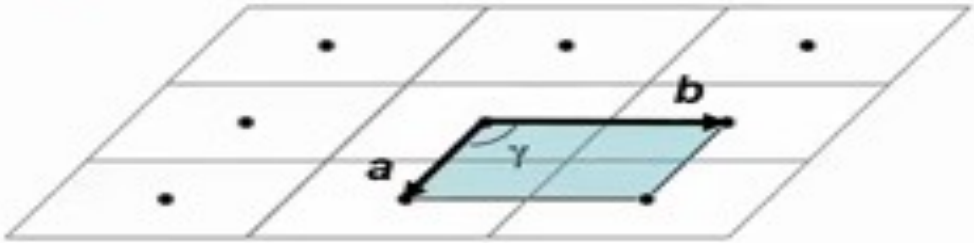

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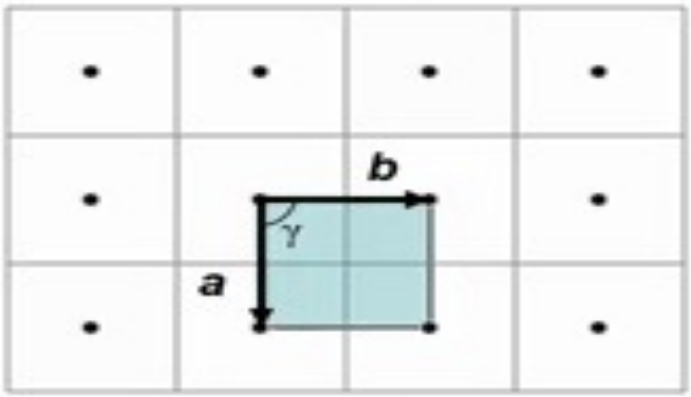
2D Crystal systems



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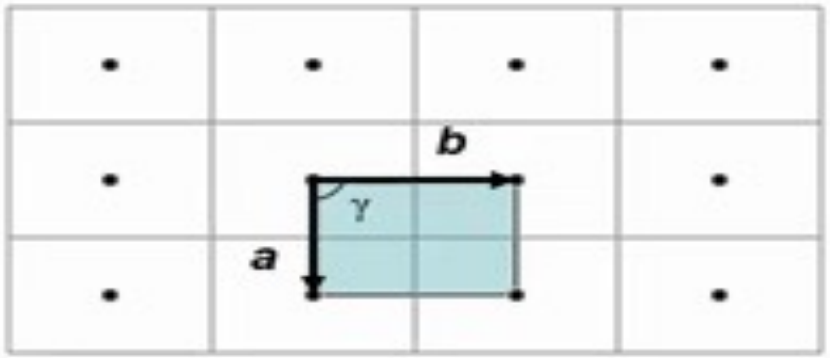

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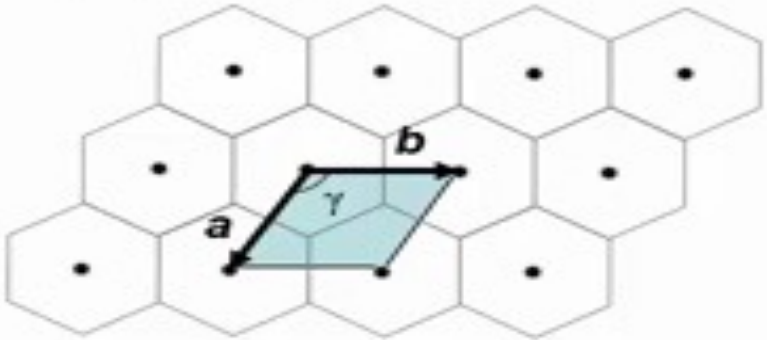

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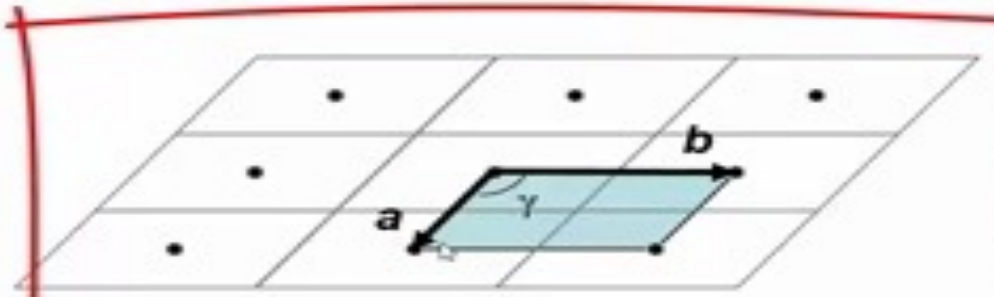

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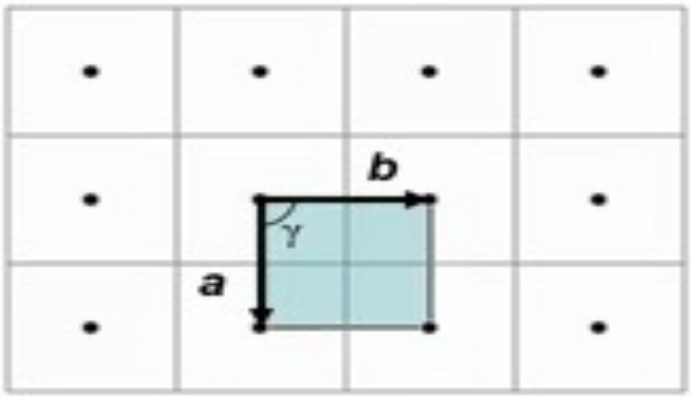

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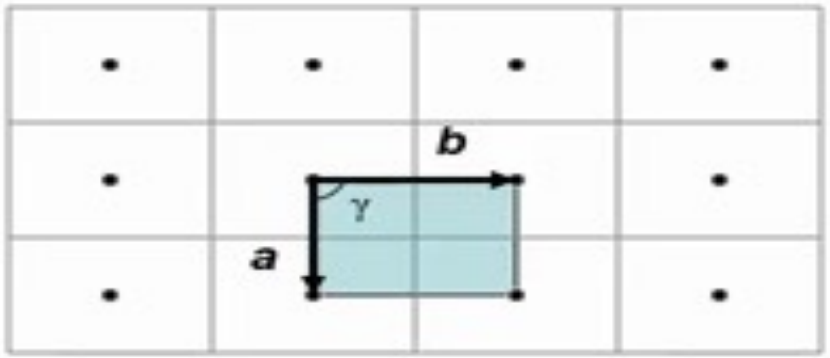

Rectangular lattice ($a \neq b$, $\gamma = 90°$)
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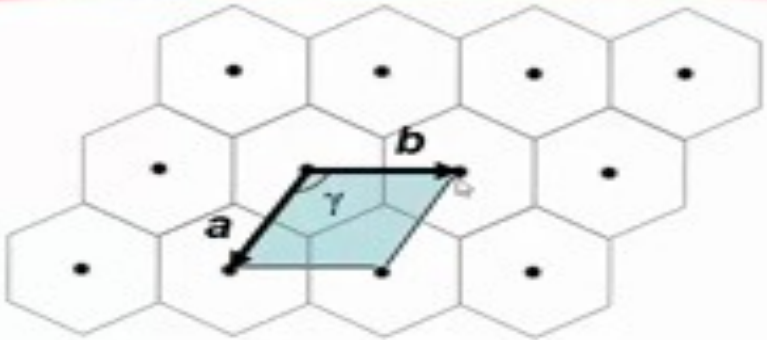

Hexagonal lattice ($a = b$, $\gamma = 120°$)
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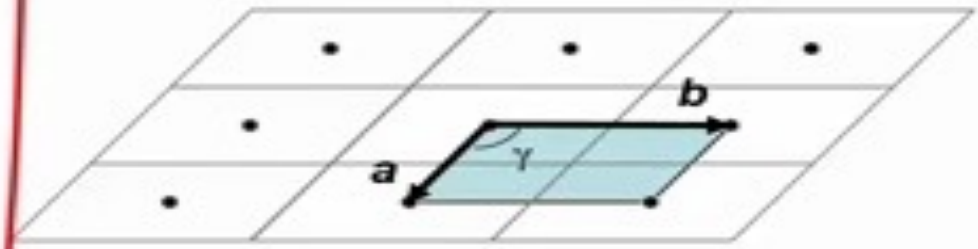

Oblique lattice ($a \neq b$, γ = arbitrary)
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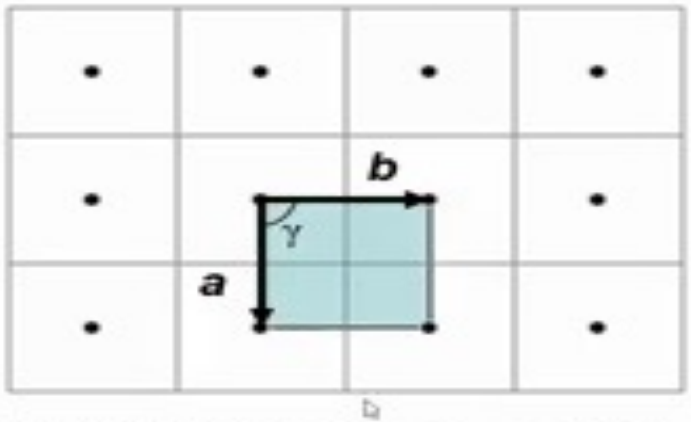
2D Crystal systems



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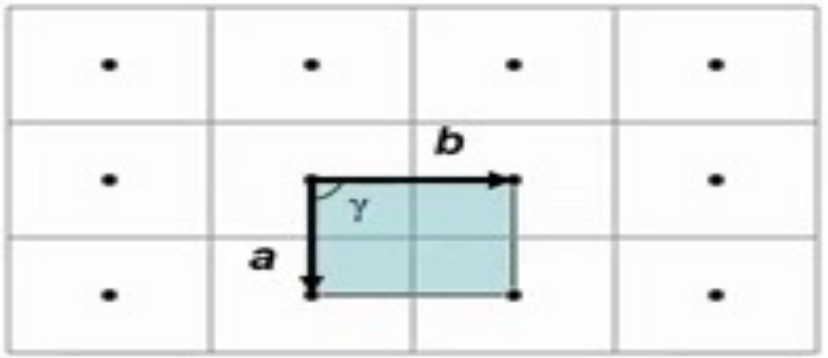

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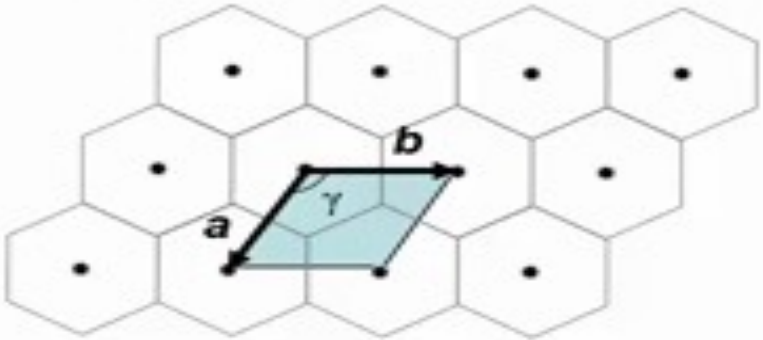

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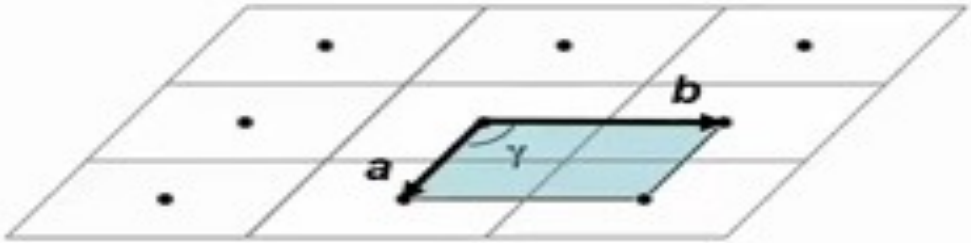
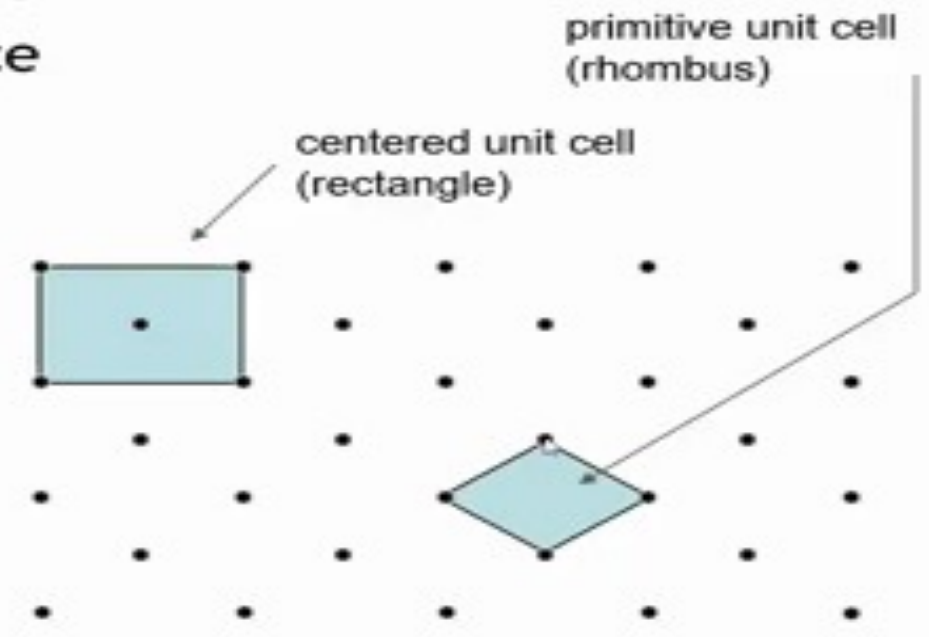


Oblique lattice ($a \neq b$, γ = arbitrary)
Req. Symmetry: None

2D Bravais Lattices

- Primitive hexagonal lattice
- Primitive square lattice
- Primitive rectangular lattice
- Centered rectangular lattice
- Primitive oblique lattice

The centered rectangular lattice contains an element of translational symmetry in addition to the lattice vectors, for every lattice point there is another at ½***a*** + ½***b***



centered rectangular lattice

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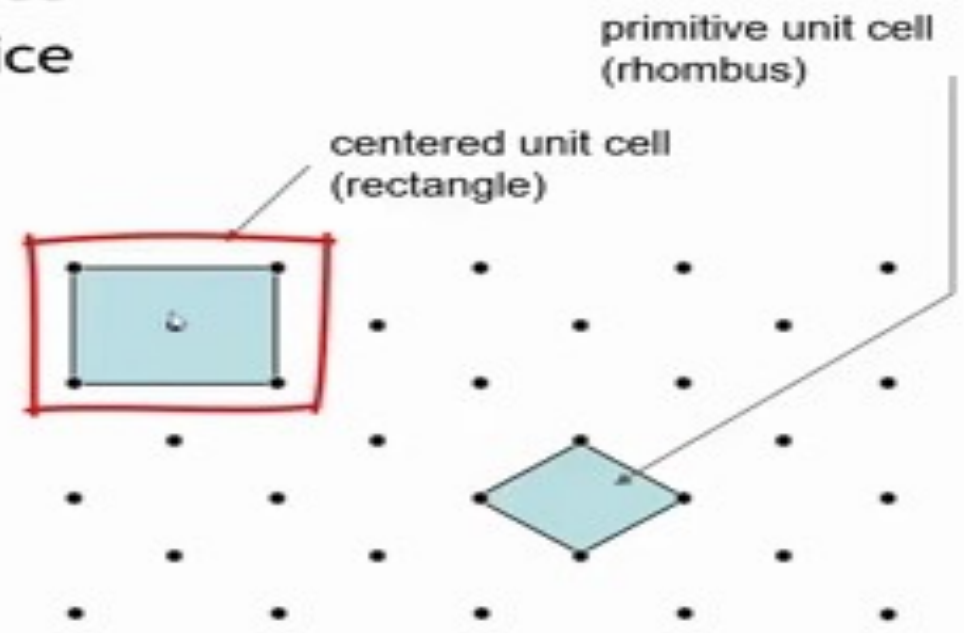

centered rectangular lattice

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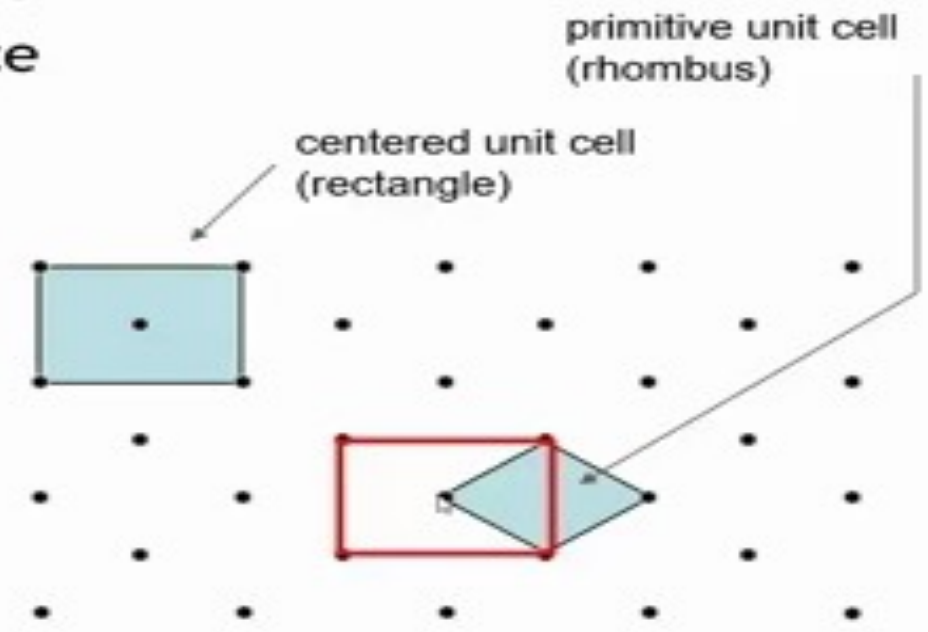

centered rectangular lattice

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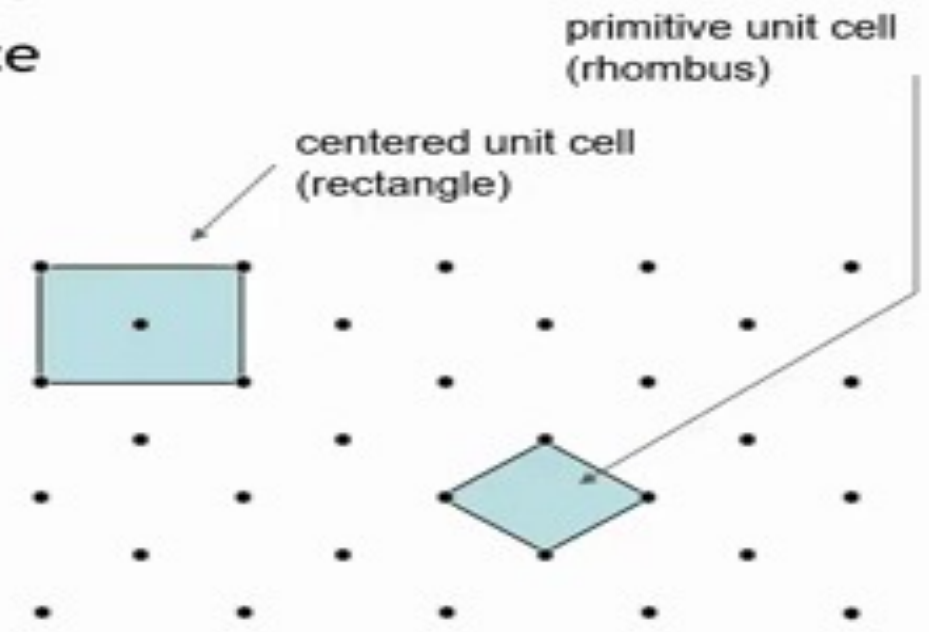
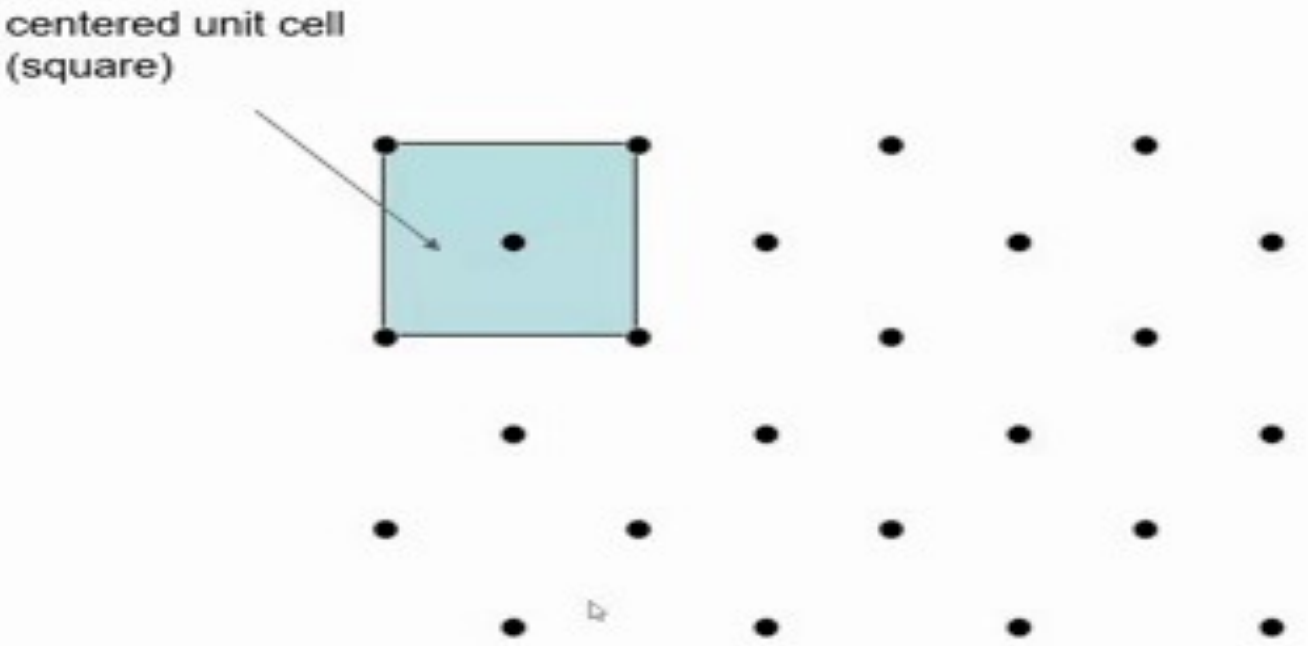


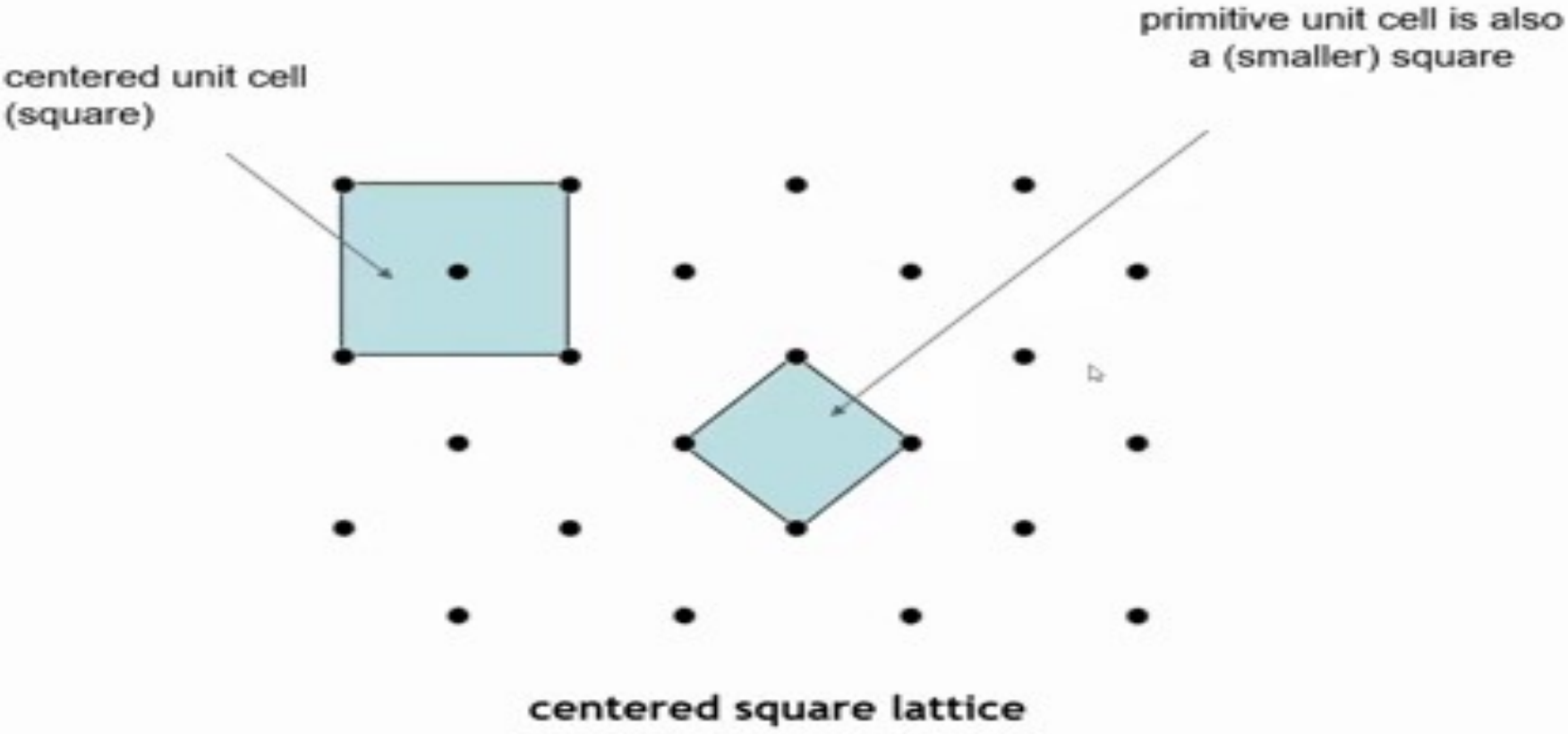
centered rectangular lattice

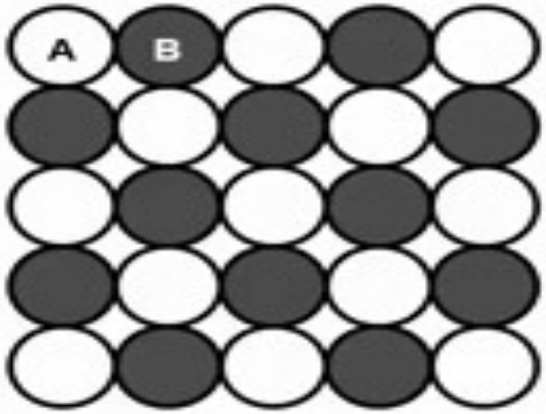
Why aren't there other centered Bravais Lattices?



centered square lattice

Why aren't there other centered Bravais Lattices?





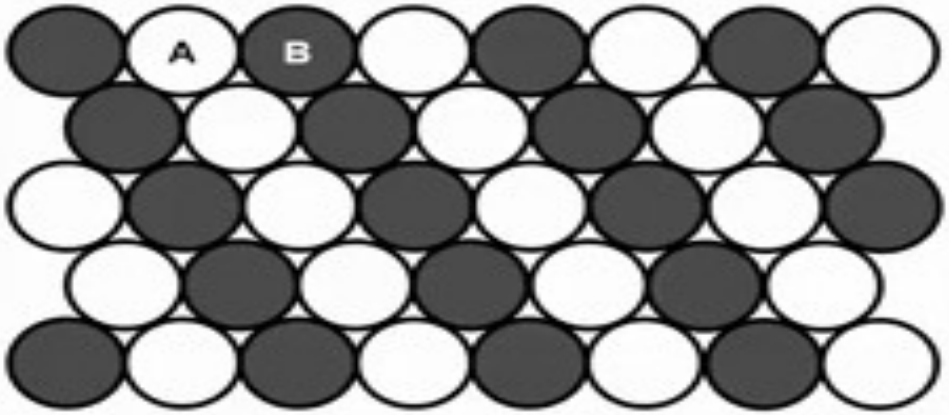
Identify the unit cell and motif

2D Bravais lattice: _____

# of atom A per unit cell: _____

# of atom B per unit cell: _____

Empirical Formula: _____



Identify the unit cell and motif

2D Bravais lattice: _____

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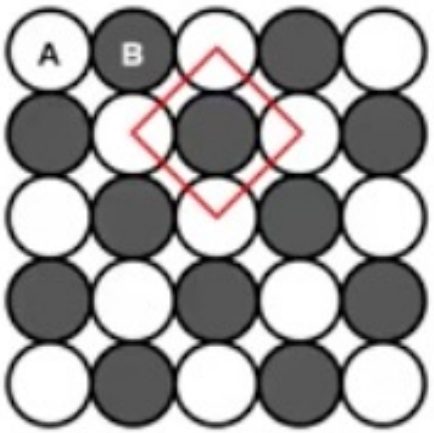


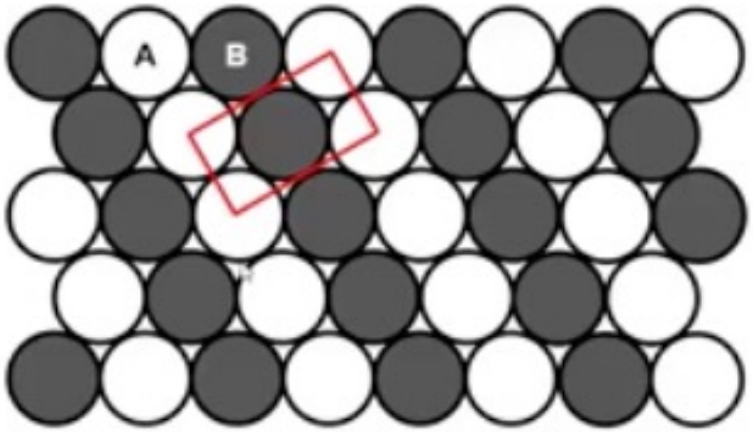
Identify the unit cell and motif

2D Bravais lattice: square

# of atom A per unit cell: 1

# of atom B per unit cell: 1

Empirical Formula: AB



Identify the unit cell and motif

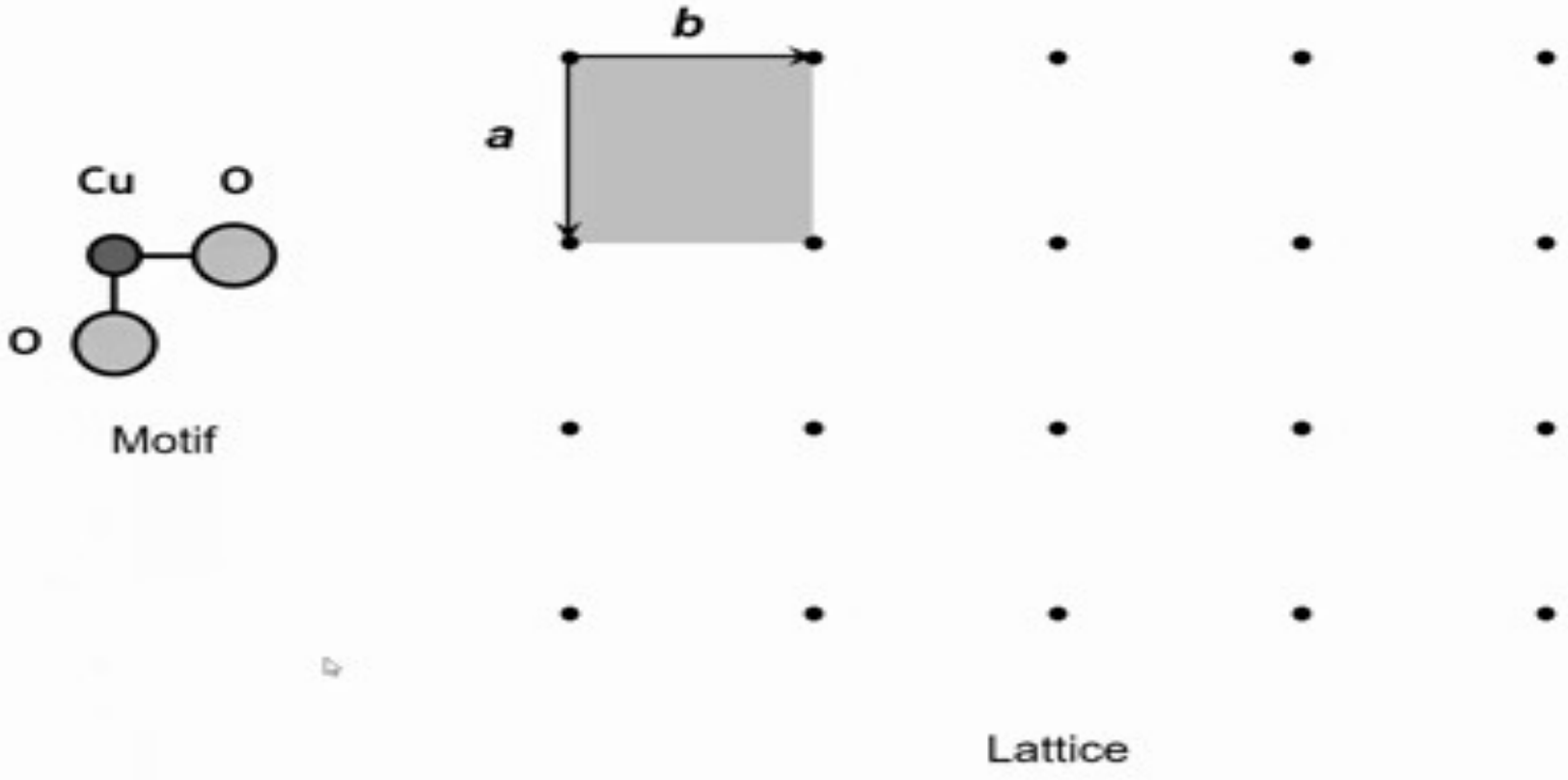
2D Bravais lattice: rectangular

# of atom A per unit cell: 1

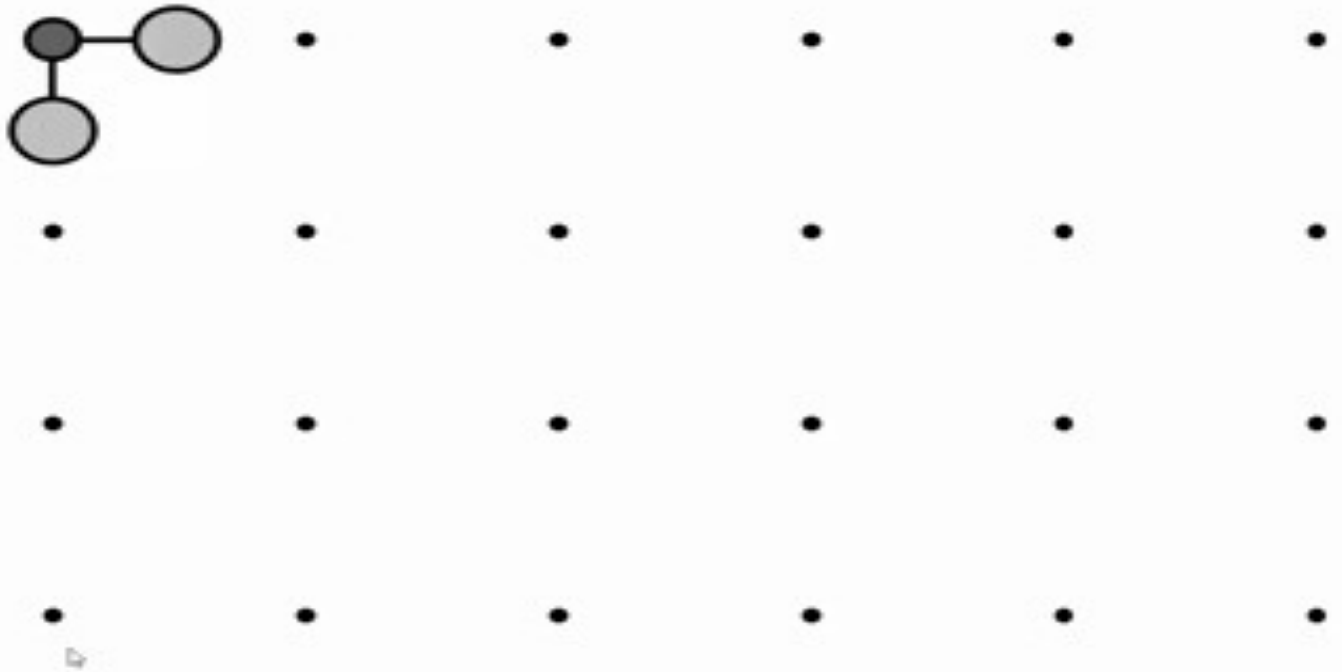
# of atom B per unit cell: 1

Empirical Formula: AB

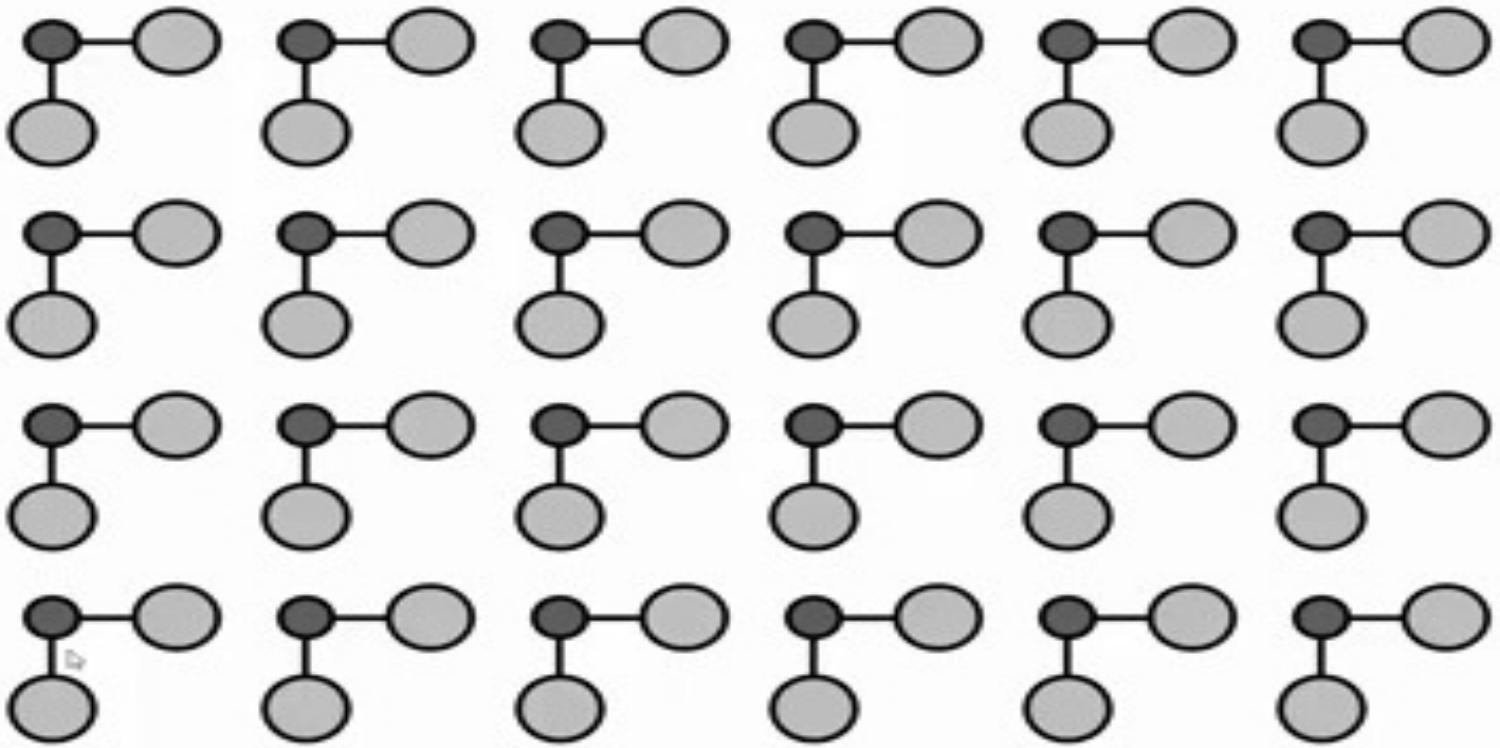
Lattice + Motif = Crystal Structure



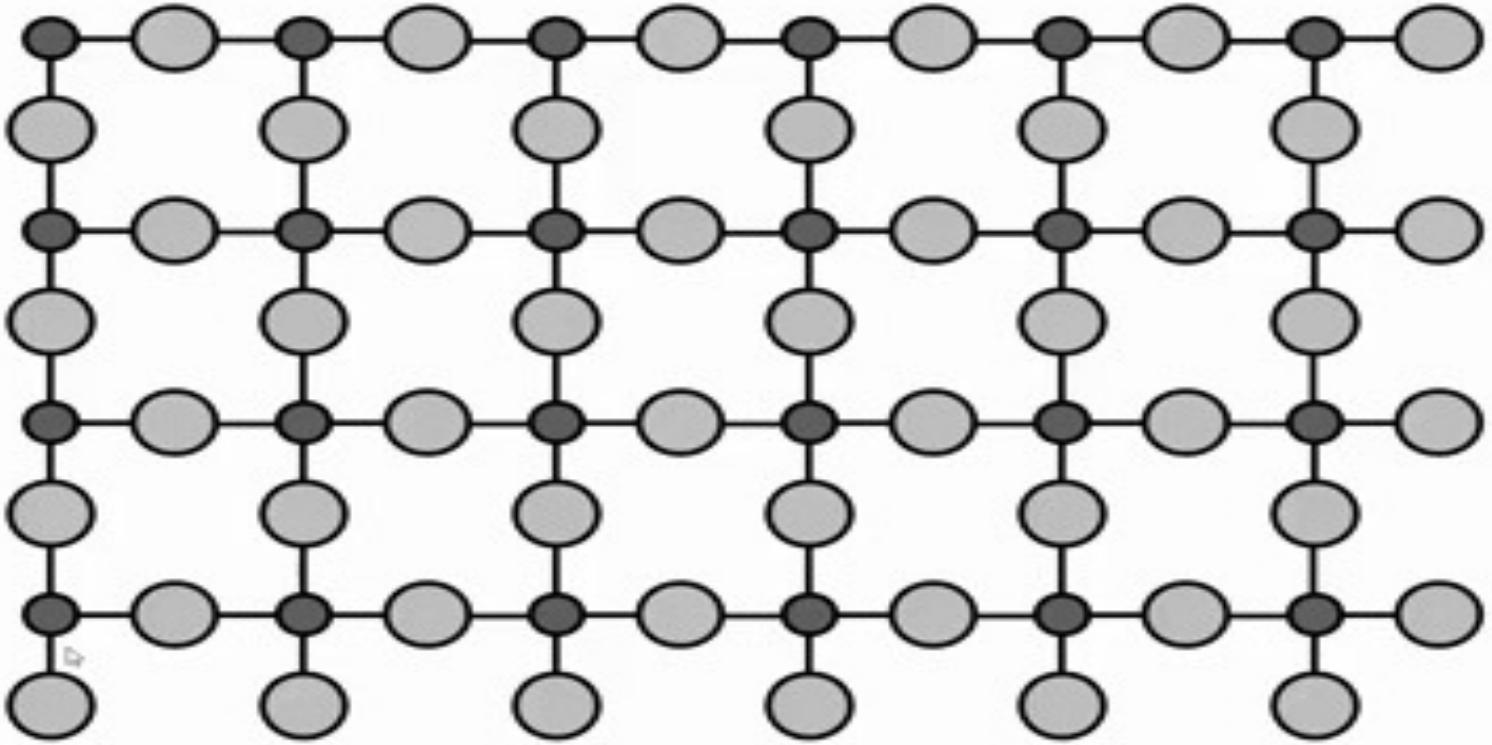
Lattice + Motif = Crystal Structure



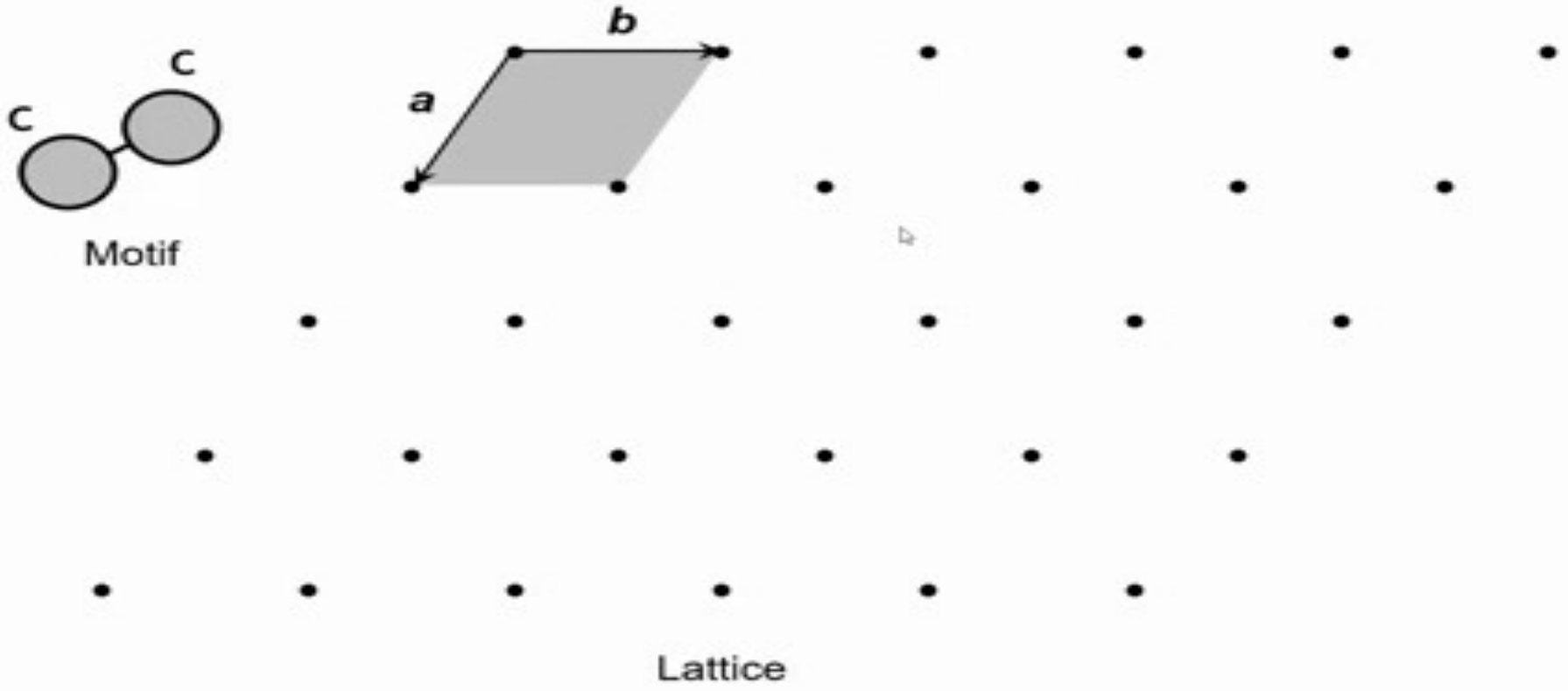
Lattice + Motif = Crystal Structure



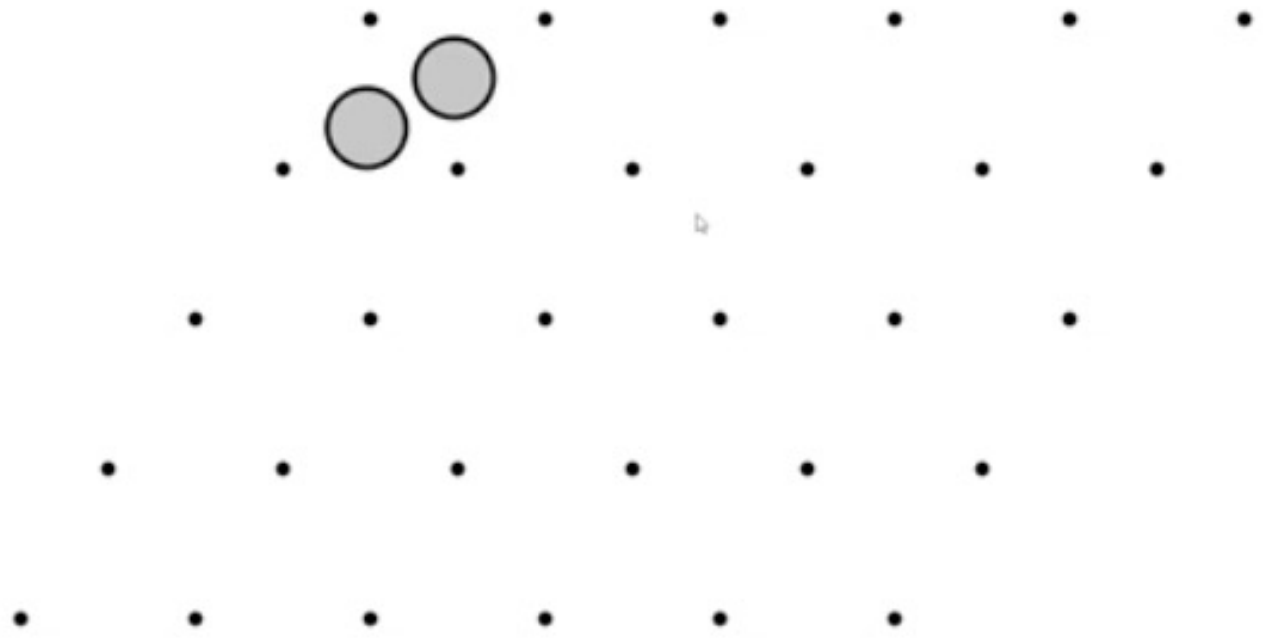
Lattice + Motif = Crystal Structure



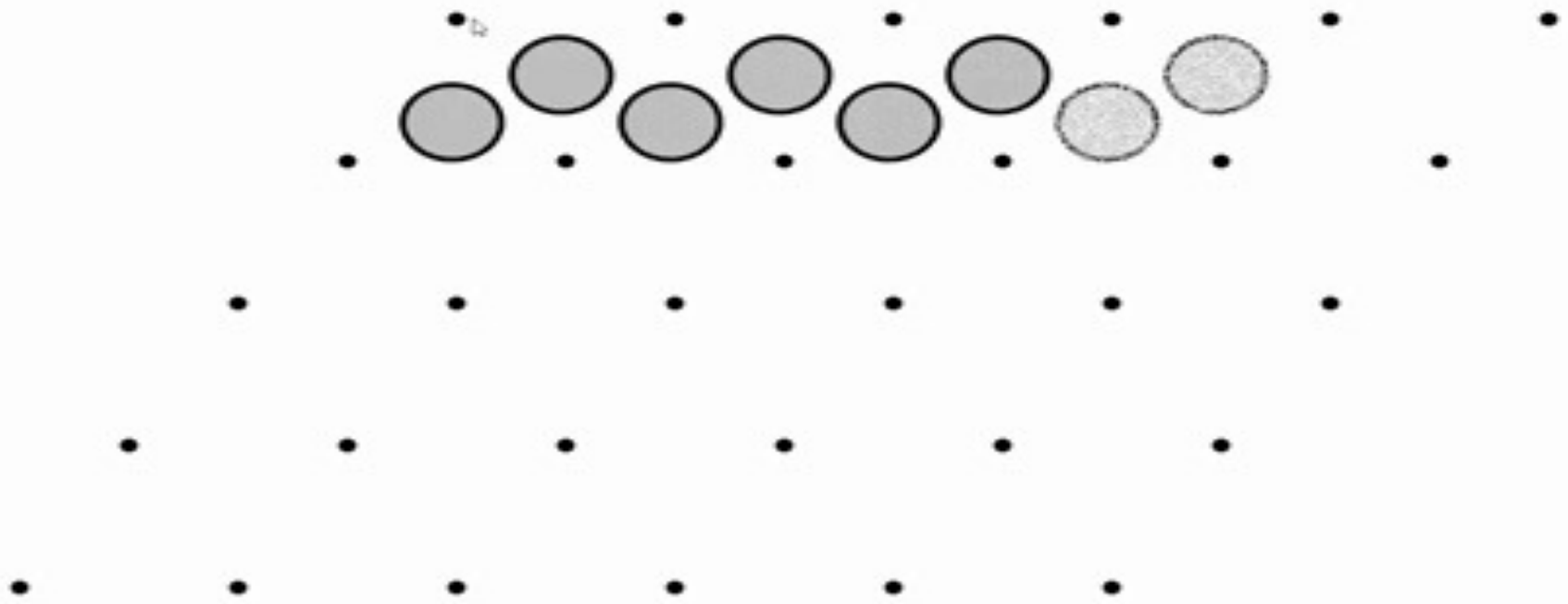
Lattice + Motif (2nd Example)



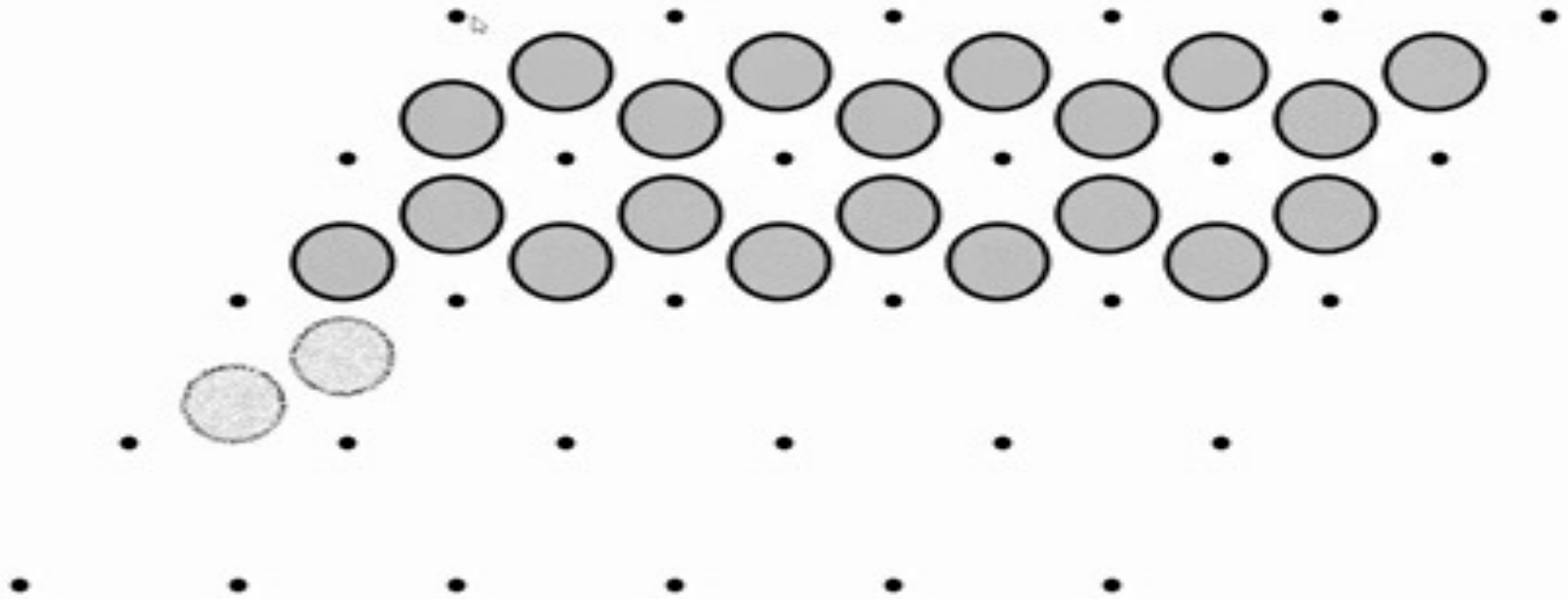
Lattice + Motif (2nd Example)



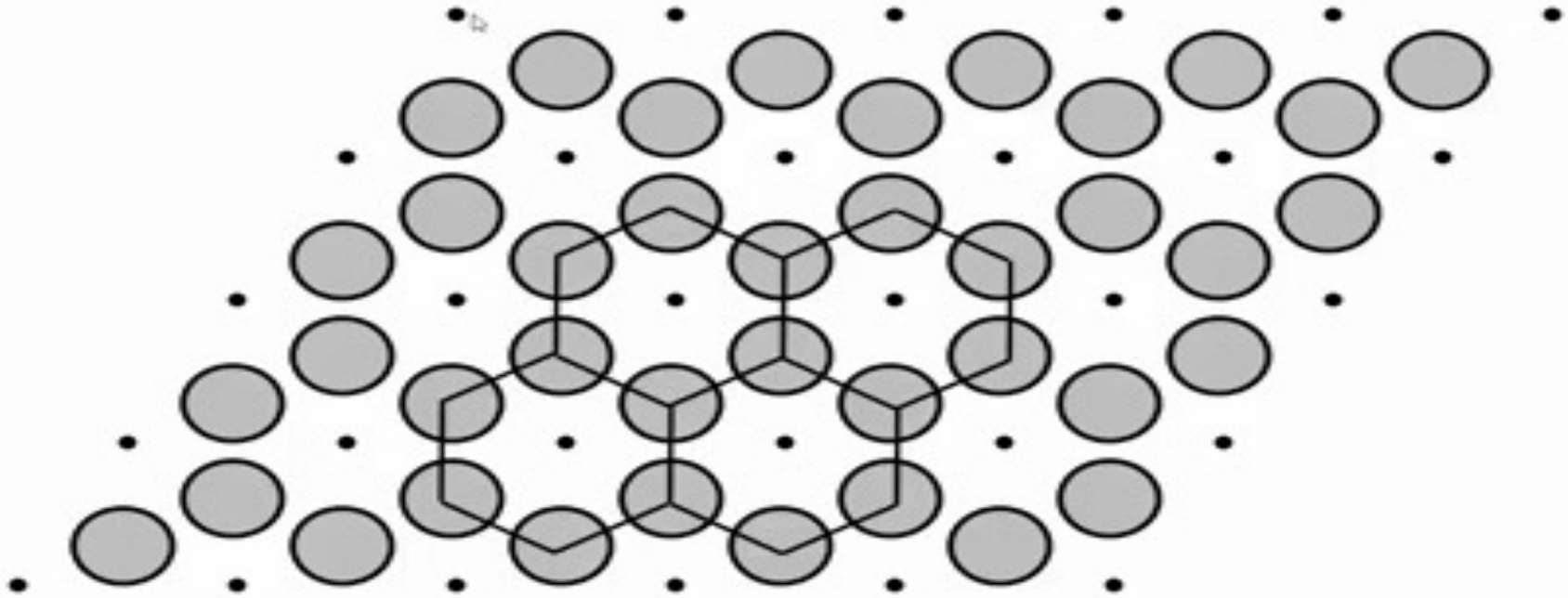
Lattice + Motif (2nd Example)

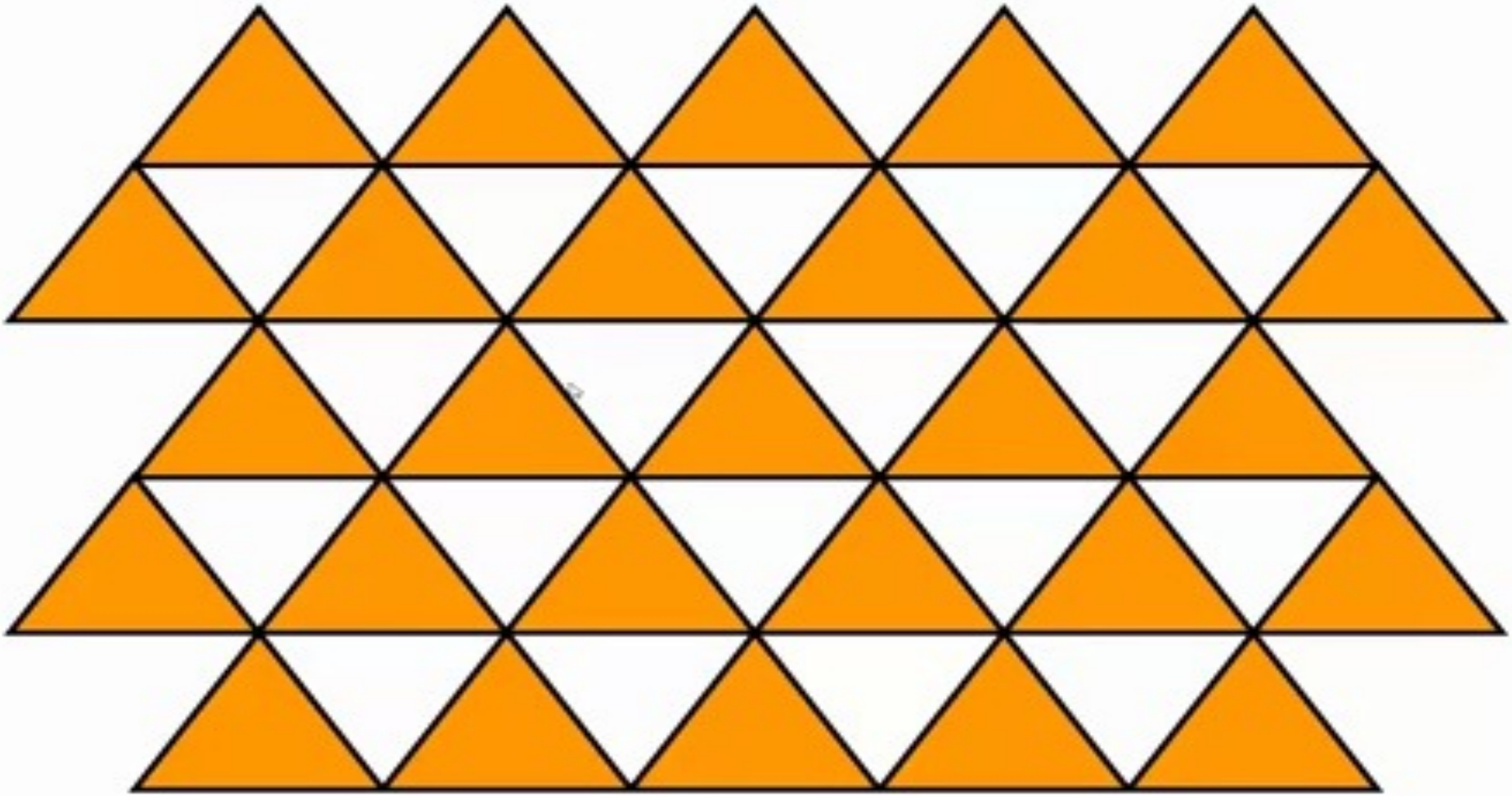


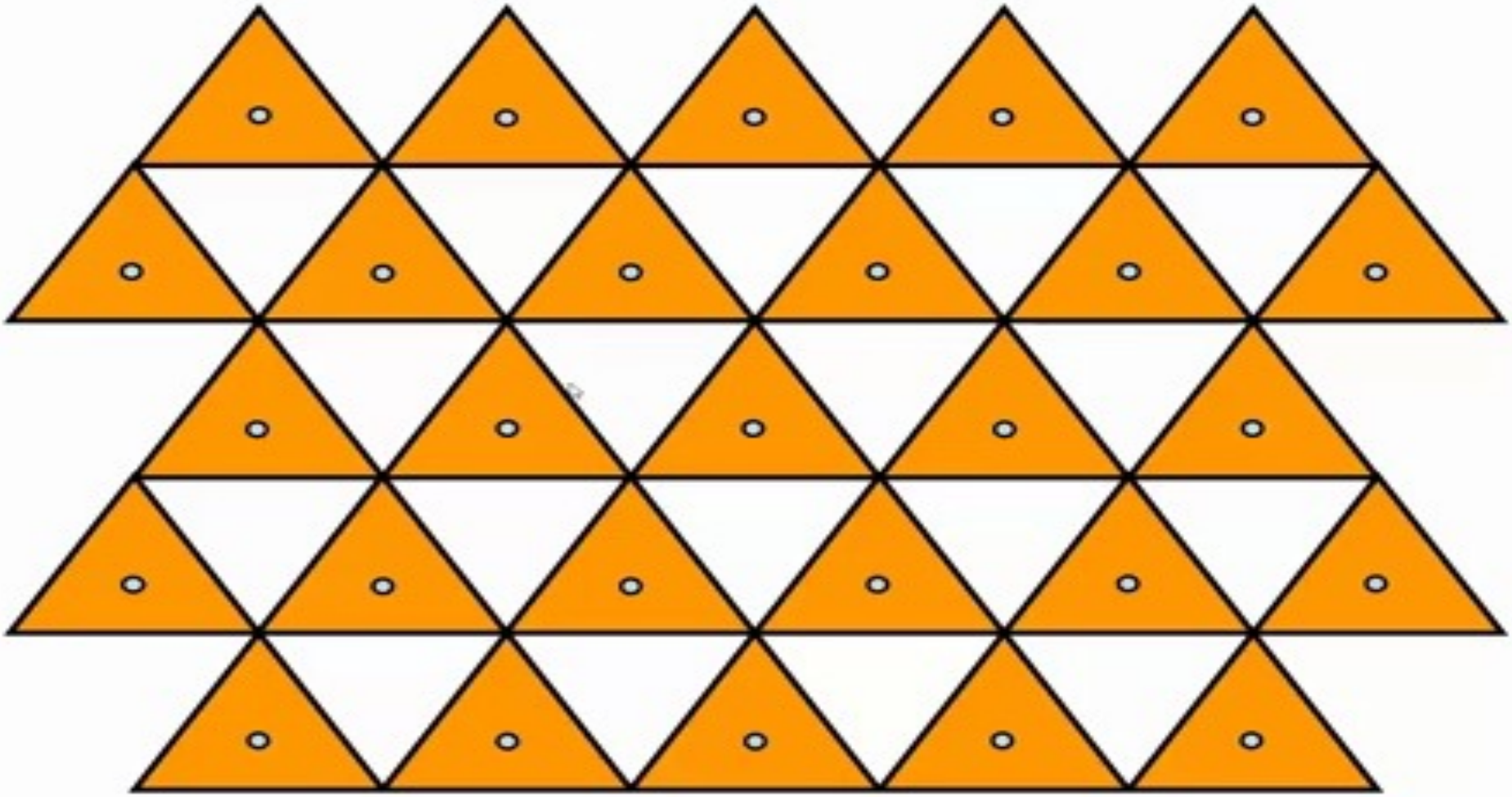
Lattice + Motif (2nd Example)

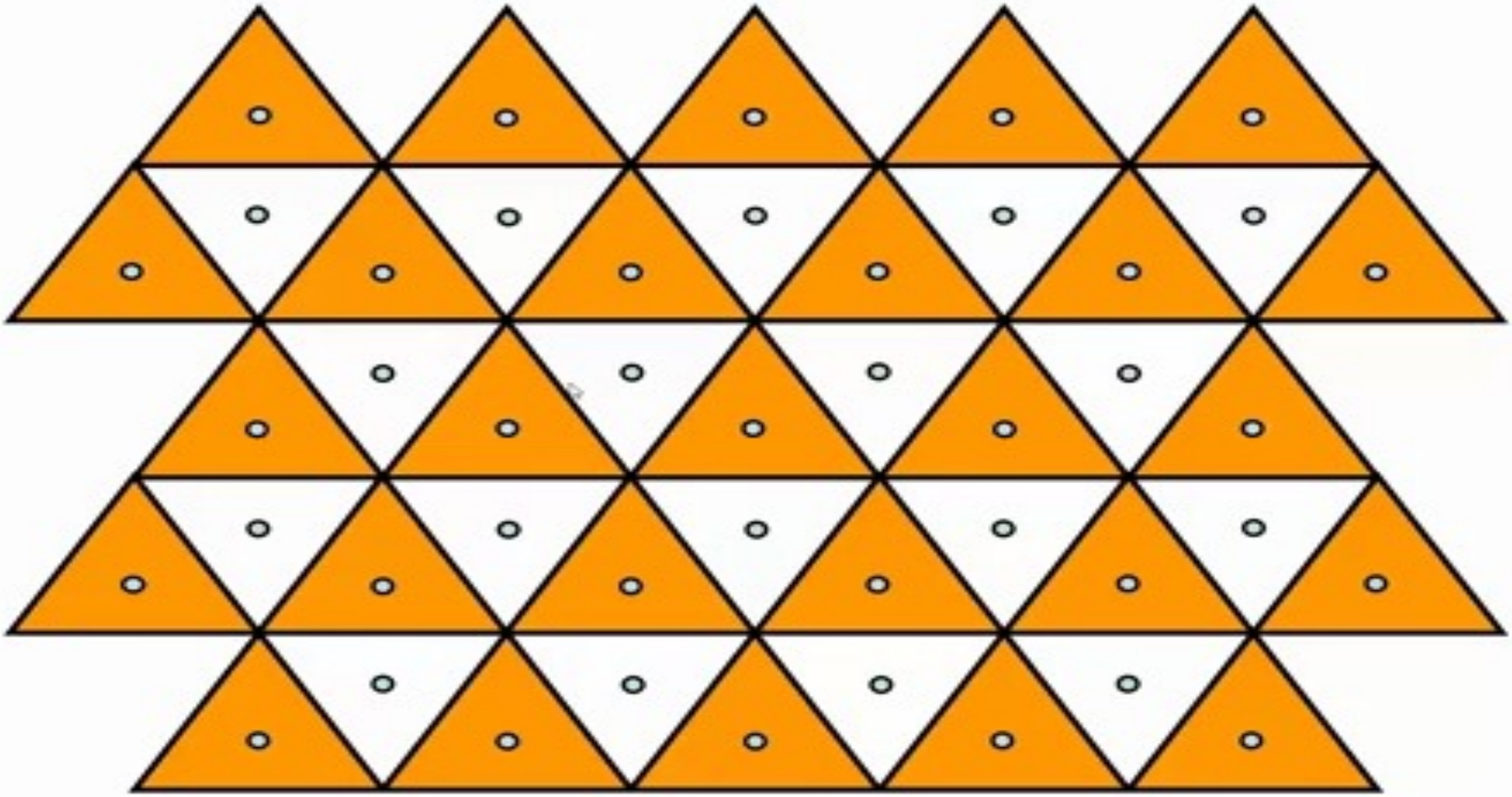


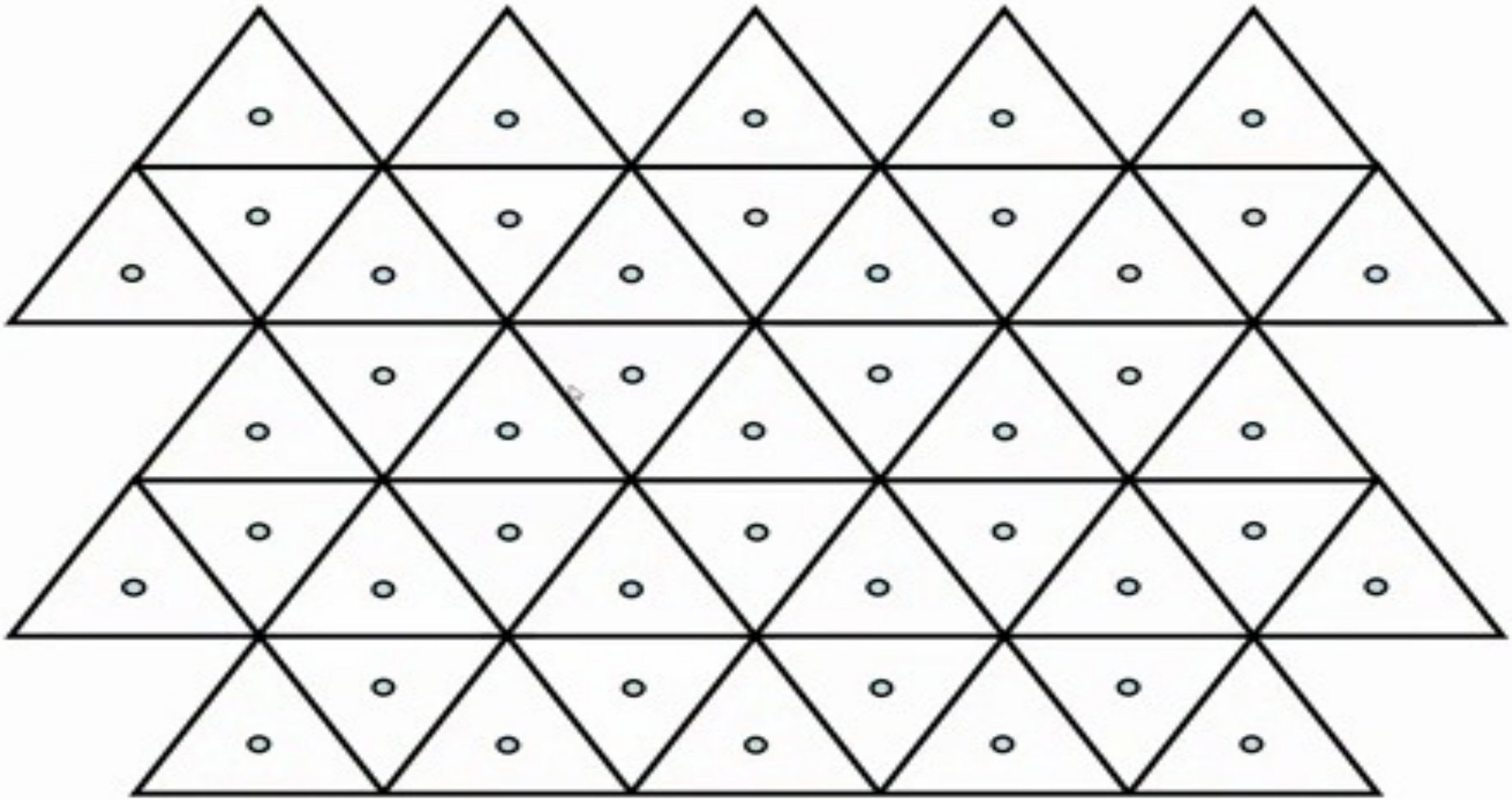
Lattice + Motif (2nd Example)

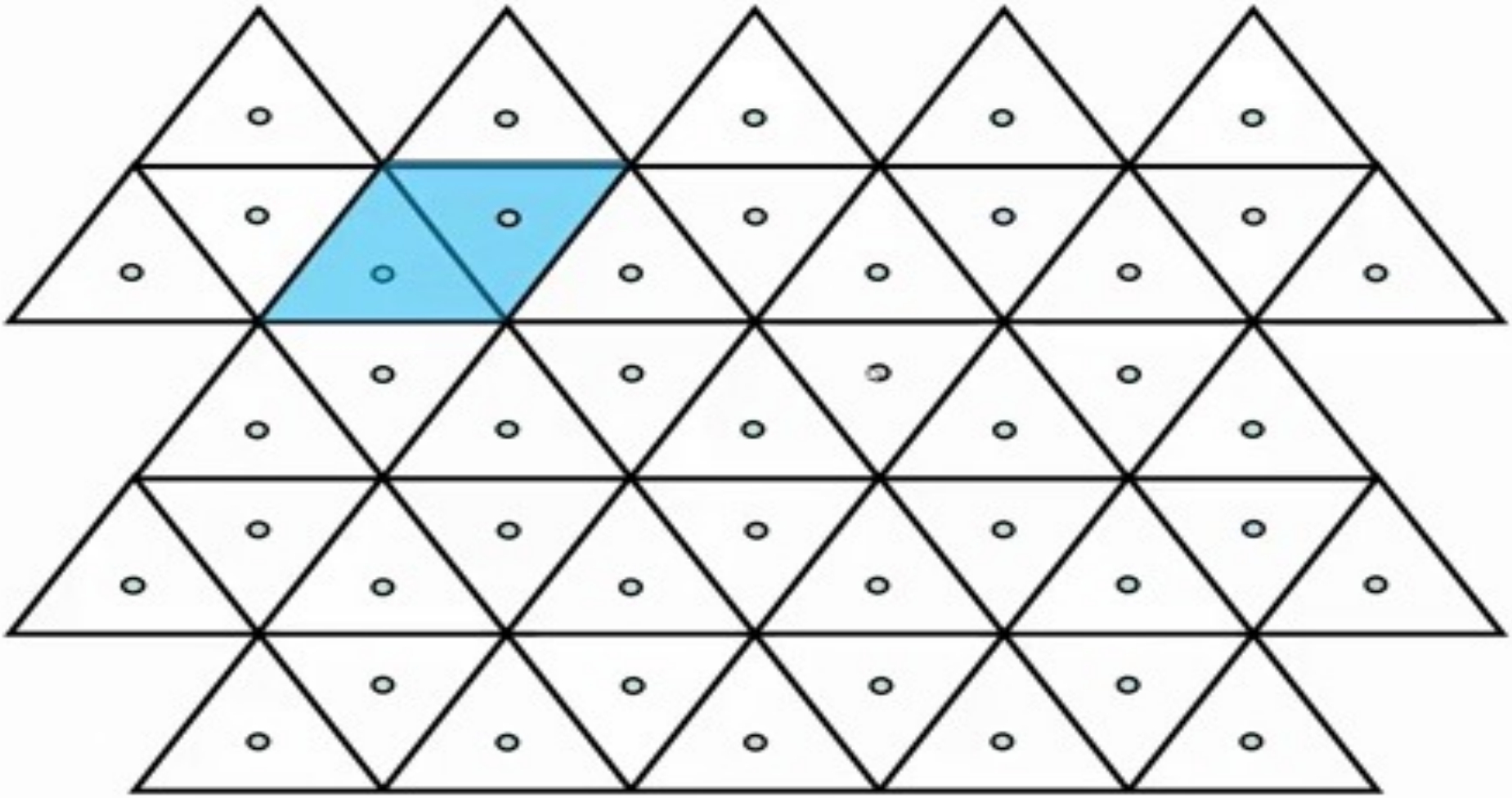












Summary — Lecture 1: Translational Symmetry in 2D

•**Two types of solids:**
•Crystalline = periodic atomic pattern
•Amorphous = no long-range order

•**Lattice + Unit Cell:**
•Lattice = infinite grid of equivalent points
•Unit cell (parallelogram in 2D) repeats to tile space

•**Which shapes/lattices tile 2D space?**
•Square, rectangle, oblique (parallelogram), hexagonal, centered rectangular

•**Symmetry Constraints:**
•Only 2-, 3-, 4-, 6-fold rotational symmetry compatible with periodic lattices

•**Motif (Basis):**
•Atoms/group of atoms attached to each lattice point
•Lattice + Motif = Crystal structure

•**Examples:**
•CuO_2 motif → layered cuprates
•2C motif in hexagonal lattice → graphene

Homework

1.2 By analogy with Table 1.1, determine the number and type of 2D crystal systems via considering their possible minimum symmetry elements and sketching their Bravais lattices.

Table 1.1 Sorting 32 crystallographic point groups into seven crystal systems.

Crystal system	Minimum symmetry	Higher-symmetry point groups
Triclinic	1	$\bar{1}$
Monoclinic	2, *m*	2/m
Orthorhombic	222	*mm*2, *mmm*
Tetragonal	4, $\bar{4}$	4/*m*, 422, 4*mm*, $\bar{4}$ 2*m*, 4/*mmm*
Hexagonal	6, $\bar{6}$	6/*m*, 622, 6*mm*, $\bar{6}$*m*2, 6/*mmm*
Trigonal	3, $\bar{3}$	32, 3*m*, $\bar{3}$*m*
Cubic	23	*m*$\bar{3}$, $\bar{4}$ 3*m*, 432, *m*$\bar{3}$*m*

Translational Symmetry in 3D

Goal:
Introduce the 3D unit cell and the classification of Bravais lattices as the foundation for describing all crystal structures.

Learning Objectives:
- Recognize the 7 crystal systems and their defining features
- Distinguish primitive, body-, face-, and base-centered lattices
- Understand how 14 Bravais lattices arise from translational symmetry

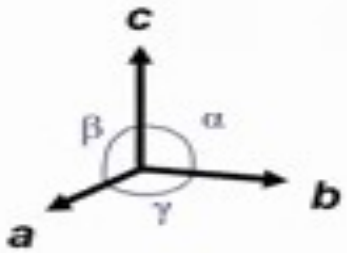
Relationship to Text:
Based on *Structures of Crystalline Materials*, Chapter 1, Section 1.1 (pp. 1–12)

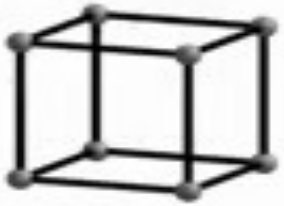
A **unit cell** is the smallest repeating **volume** that can be translated through space (by lattice vectors) to build the entire crystal lattice.

•In **2D**, the unit cell is an area (a parallelogram).

•In **3D**, it's a volume (a **parallelepiped** — six faces, opposite faces parallel, each face a parallelogram).

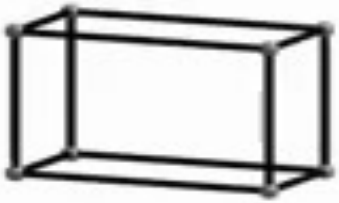
3D Unit Cells





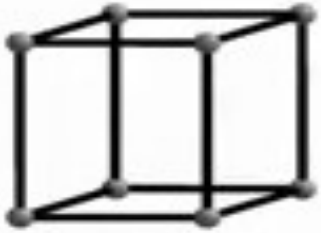
Cubic
a = b = c
α = β = γ = 90°

Tetragonal
a = b ≠ c
α = β = γ = 90°

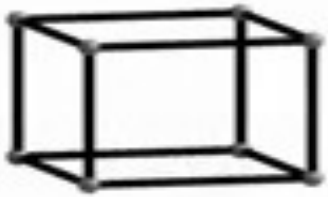


Orthorhombic
a ≠ b ≠ c
α = β = γ = 90°

Rhombohedral
a = b = c
α = β = γ ≠ 90°



Hexagonal
a = b ≠ c
α = β = 90°, γ = 120°



Monoclinic
a ≠ b ≠ c
α = γ = 90°, β ≠ 90°

Triclinic
a ≠ b ≠ c
α ≠ β ≠ γ

Lattice centering tells us how many **lattice points** are inside a chosen **unit cell** (beyond just the corners).
•A **primitive (P) unit cell** has **only corner lattice points**, which add up to exactly 1 lattice point per cell.
•A **centered unit cell** has additional lattice points located inside the cell (body center or face centers).

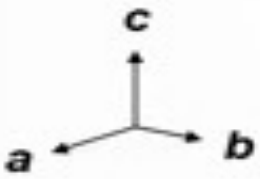
These are not "extra atoms" — they're just extra **repeat positions** that fall inside the boundaries of that particular choice of unit cell.

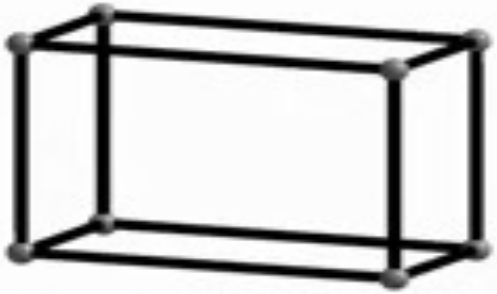
A **lattice point** is an abstract point in space that marks the repeating positions of the crystal pattern.
•Mathematically, every lattice point is generated by:

$$\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3, \quad n_i \in \mathbb{Z}.$$

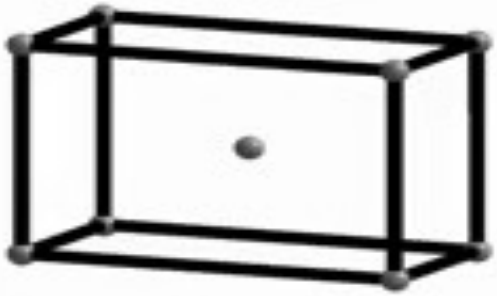
•Physically, you don't put a single atom at a lattice point necessarily. Instead, you attach a **motif** (an atom, group of atoms, or molecule) to *every* lattice point. The whole crystal is then the lattice + motif.

Lattice Centering

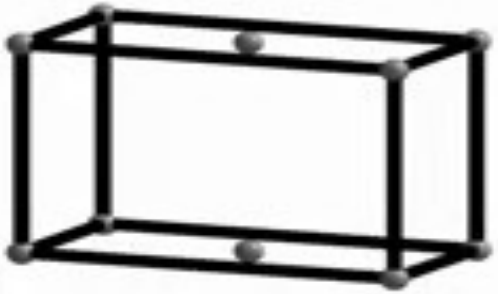




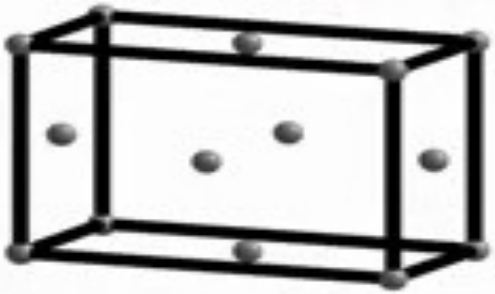
Primitive lattice (P)
no centering



Body centered lattice (I)
*For every atom there is another at ½**a** + ½**b** + ½**c***



Base centered lattice (C)
*For every atom there is another at ½**a** + ½**b***



Face centered lattice (F)
For every atom there are 3 more at:
*½**a** + ½**b***
*½**a** + ½**c***
*½**b** + ½**c***

Bravais lattice = infinite set of equivalent points

A **Bravais lattice** is the set of all points generated by integer linear combinations of a primitive set of **lattice vectors**:

$$\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3, \quad n_i \in \mathbb{Z}.$$

Different primitive choices of $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ can generate the *same lattice*. The lattice is the point set, not the cell we draw.

The 14 Bravais lattices are the irreproducible building blocks of all 3D crystals.

Rules for a Bravais lattice

Translational Equivalence
Every lattice point must be identical (equivalent environment) when shifted by an integer combination of lattice vectors.

Minimal Cell (Primitive Cell Exists)
You cannot define a larger "centered" cell if a smaller primitive cell generates the same lattice more simply.
→ Redundant centerings are thrown out.

Consistency with Crystal System Symmetry
The Bravais lattice must obey the symmetry constraints of its crystal system (e.g., cubic requires all edges equal, all angles 90°).
→ Some centering choices break the system's symmetry and therefore aren't distinct.

There are 7 crystal systems × 4 possible centering types (primitive P, body I, face F, base C) = 28 candidates.
But many are duplicates or impossible under the rules above:

Crystal system	Possible centerings	Allowed Bravais lattices	Why others are excluded
Triclinic	P, I, F, C	**P only**	Any centering can be reduced to a primitive cell.
Monoclinic	P, I, F, C	**P, C**	I and F reduce to C (not unique).
Orthorhombic	P, I, F, C	**P, C, I, F**	All four are distinct here.
Tetragonal	P, I, F, C	**P, I**	F and C reduce to P.
Cubic	P, I, F, C	**P, I, F**	C reduces to P.
Hexagonal	P, I, F, C	**P only**	Centerings reduce to primitive hexagonal.
Rhombohedral	P, I, F, C	**R only**	"R" (rhombohedral) is distinct; other centering labels reduce to R.

Fourteen 3D Bravais Lattices

Crystal System	P	C	I	F	Examples
Triclinic ($a \neq b \neq c$; $\alpha \neq \beta \neq \gamma$)	X				Primitive triclinic
Monoclinic ($a \neq b \neq c$; $\alpha = \gamma = 90^\circ$ $\beta \neq 90$)	X	X			Base-centered monoclinic
Orthorhombic ($a \neq b \neq c$; $\alpha = \beta = \gamma = 90^\circ$)	X	X	X	X	Face-centered orthorhombic
Rhombohedral ($a = b = c$; $\alpha = \beta = \gamma \neq 90^\circ$)	X				Primitive rhombohedral
Hexagonal ($a = b \neq c$; $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$)	X				Primitive hexagonal
Tetragonal ($a = b \neq c$; $\alpha = \beta = \gamma = 90^\circ$)	X		X		Body-centered tetragonal
Cubic ($a = b = c$; $\alpha = \beta = \gamma = 90^\circ$)	X		X	X	Face-centered cubic

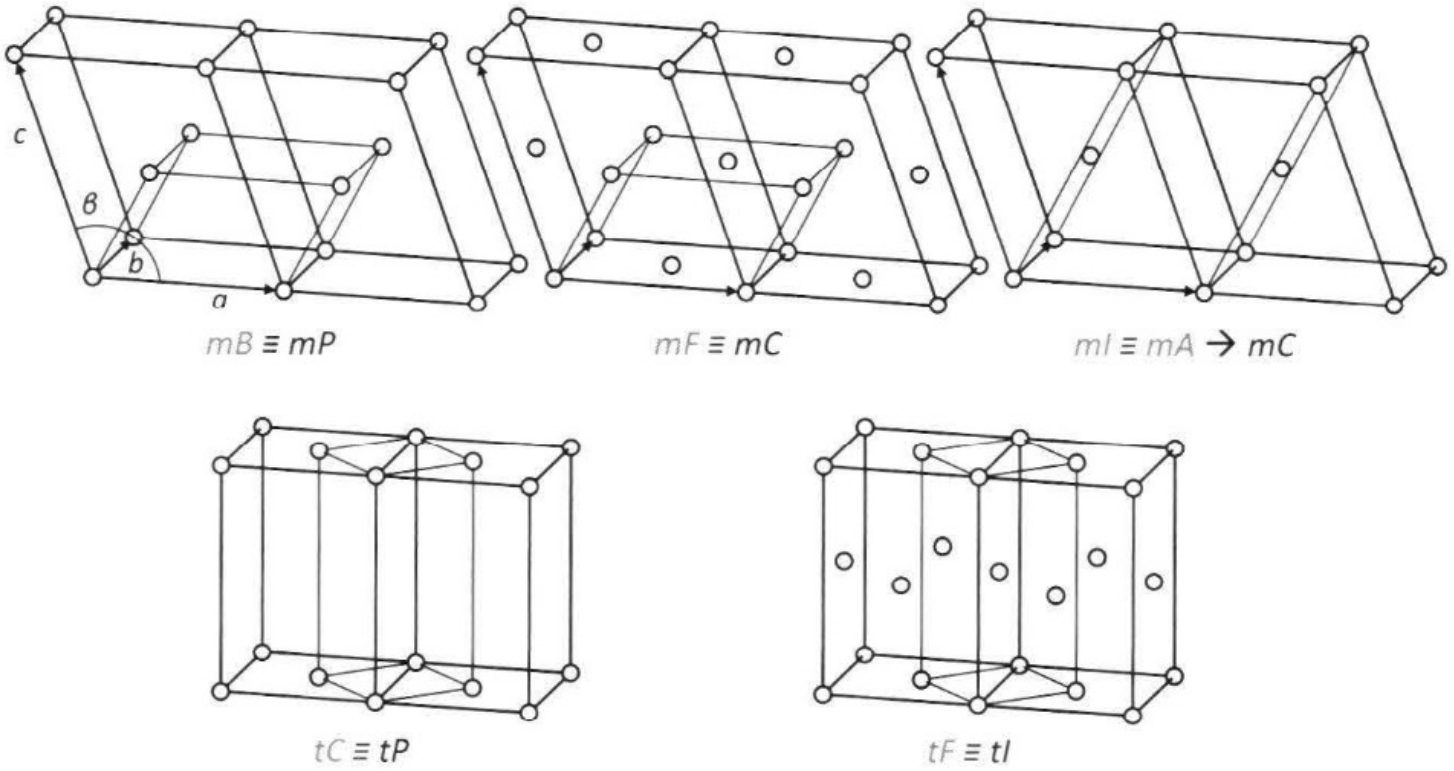
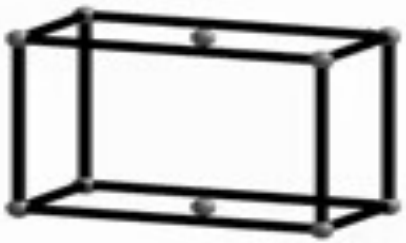


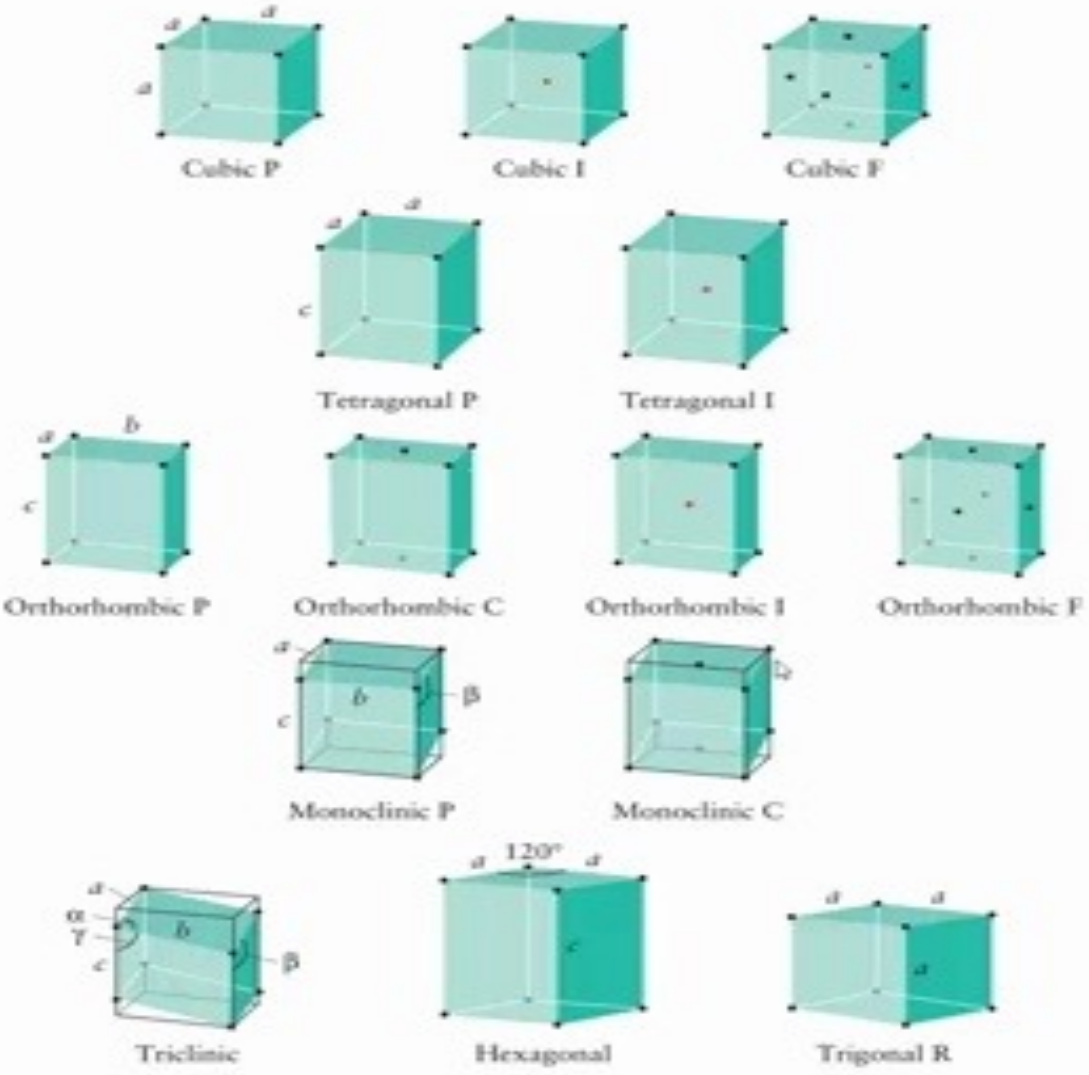
Figure 1.7 Non-standard centering of monoclinic (top) and tetragonal Bravais cells (bottom). Drawing two cells reveals the true cell of the same crystal system.

The 14 3D Bravais Lattices

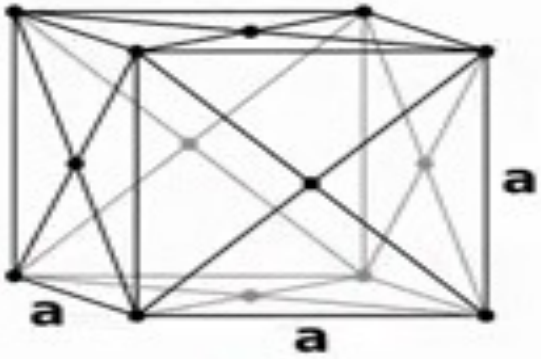
P = Primitive lattice
I = Body centered lattice
F = Face centered lattice
C = Base centered lattice



Bace-centered lattice

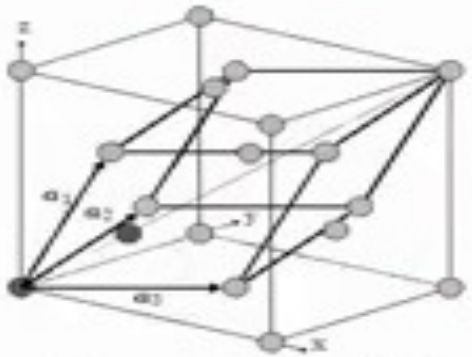


Centered and Primitive Unit Cells



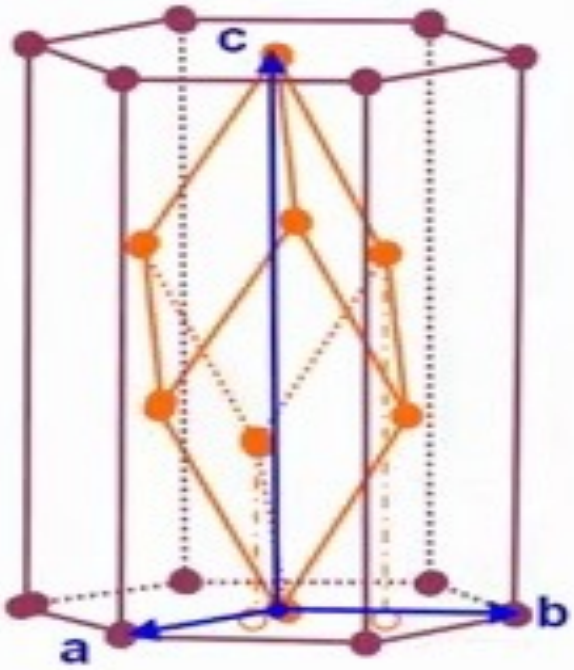
cell edge = a_{cubic}

$\alpha = \beta = \gamma = 90°$



$a_{primitive} = a_{cubic}/\sqrt{2}$

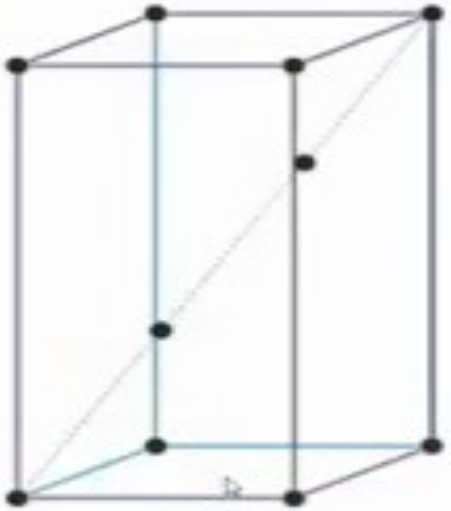
$\alpha = \beta = \gamma = 60°$



Primitive rhombohedral

&

R-centered hexagonal



For every atom there are 2 more at

2/3 ***a*** + 1/3 ***b*** + 1/3 ***c***

1/3 ***a*** + 2/3 ***b*** + 2/3 ***c***

Slide Title: Summary – Translational Symmetry in 3D

Key Points:

•A 3D crystal is built by repeating a **unit cell** (a parallelepiped) through translational symmetry.

•**Seven crystal systems**: cubic, tetragonal, orthorhombic, rhombohedral, hexagonal, monoclinic, triclinic.

•**Centered lattices**: primitive (P), body-centered (I), face-centered (F), base-centered (A, B, C).

•Combining systems + centering gives the **14 Bravais lattices**, the complete set of 3D lattice types.

•This framework underpins all crystallography: every crystal structure belongs to one of these lattices.

Homework:

Consider the cubic crystal system. Why is there **no distinct "base-centered cubic" lattice**?