

Jan-9-2013

PHYS 342/555
Introduction to solid state physics

Instructor: Dr. Pengcheng Dai
Professor of Physics
The University of Tennessee
(Room 407A, Nielsen, 974-1509)
(Office hours: TR 1:10PM-2:00 PM)
Lecture 2, room 306 Nielsen
Chapter 2: Crystal Structures
Lecture in pdf format will be available at:
<http://www.phys.utk.edu>

Solid or Condensed

- Solid state physics
- condensed matter physics
- SSP is the applied physics associated with technology rather than interesting fundamentals

Acknowledge

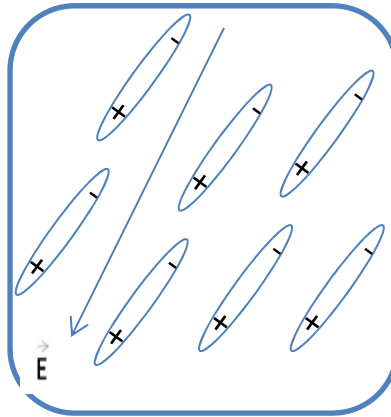
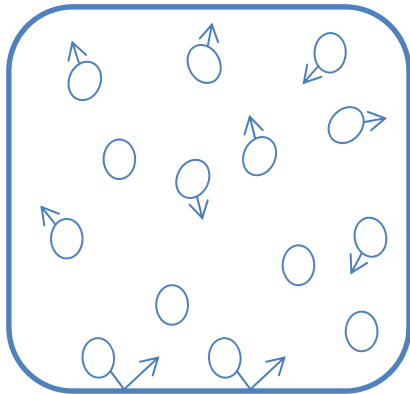
- Pengcheng's slides
- Prof.Dr.Besire Gonul
- Wikipedia
- others

MATTER

GASES

LIQUIDS
AND LIQUID
CRYSTALS

SOLIDS

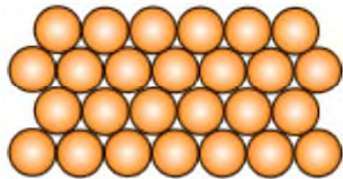
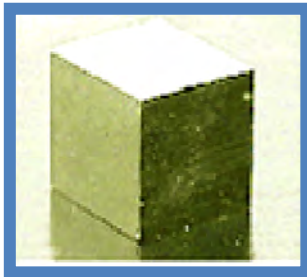


?

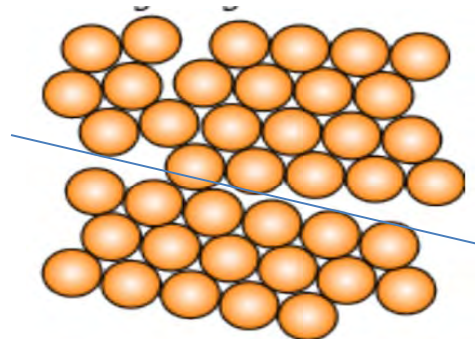
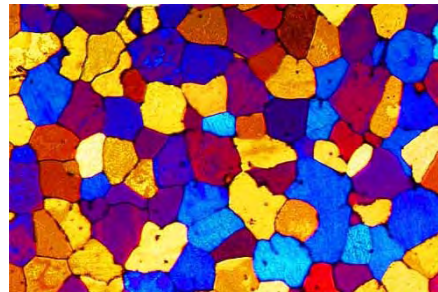
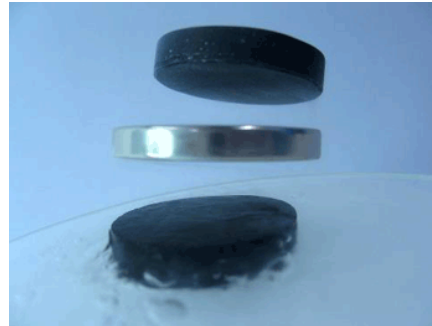
SOLID MATERIALS

CRYSTALLINE

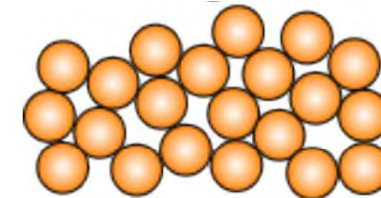
Single Crystal



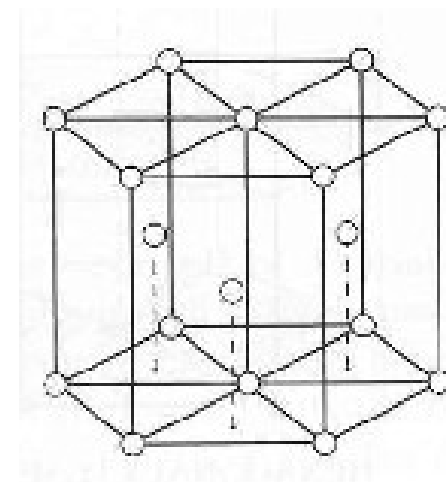
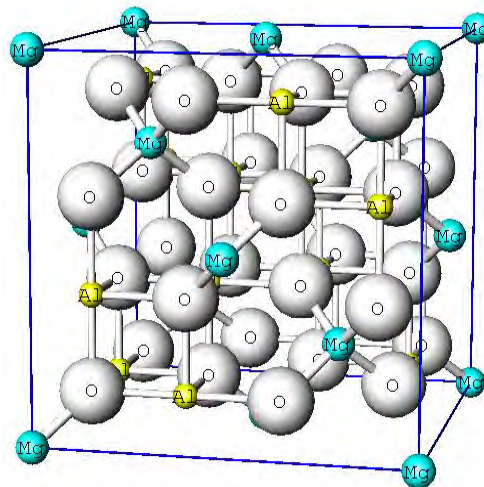
POLYCRYSTALLINE



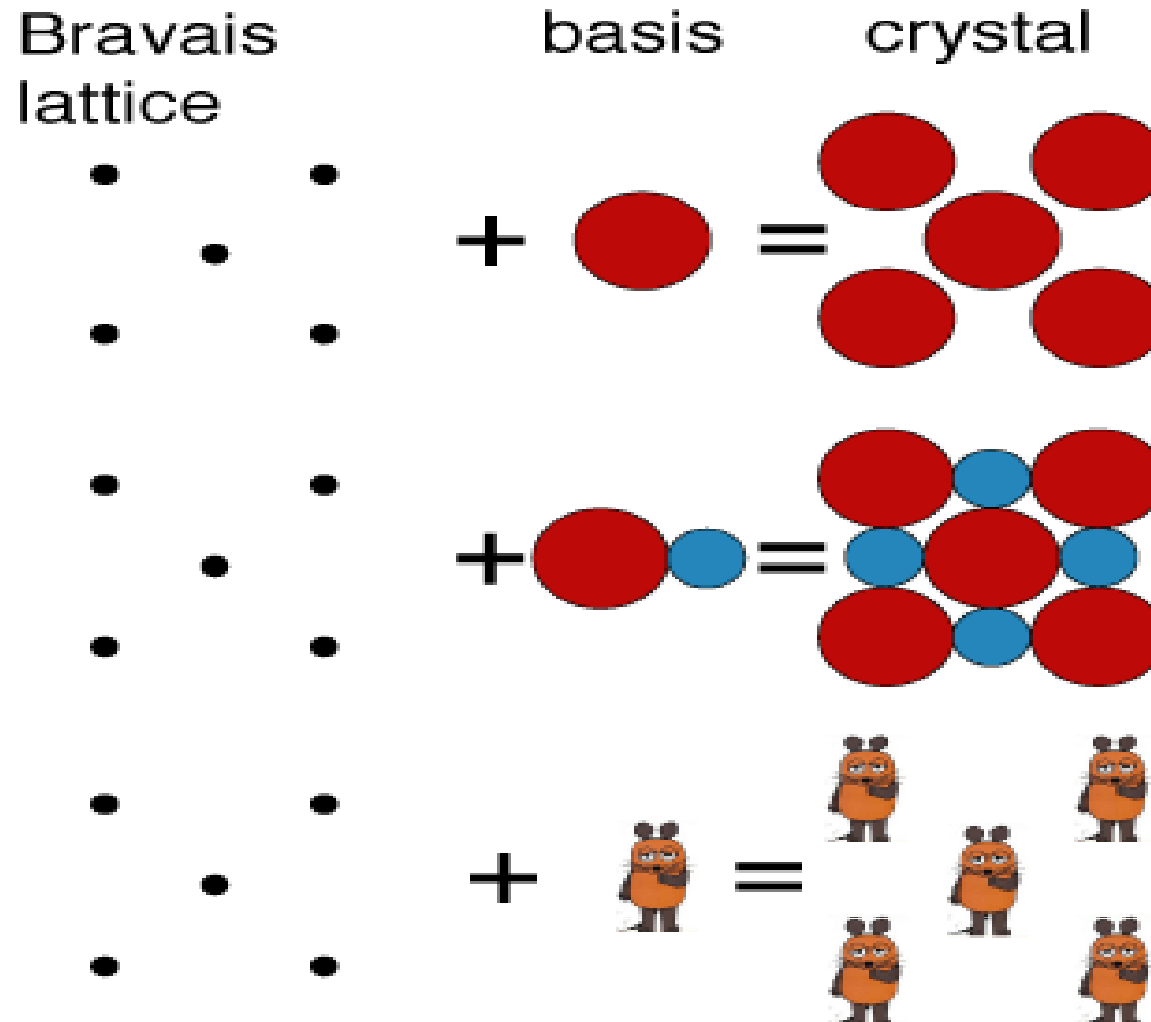
**AMORPHOUS
(Non-crystalline)**



Crystal Shape?



Bravais Lattice



Bravais Lattice

1, An array of points such that every point has *identical surroundings*

2, *primitive lattice: (a minimum-volume unit cell)*

3, *position vector:*

$$\vec{R} = n_1 \vec{a}_1 \quad (1D)$$

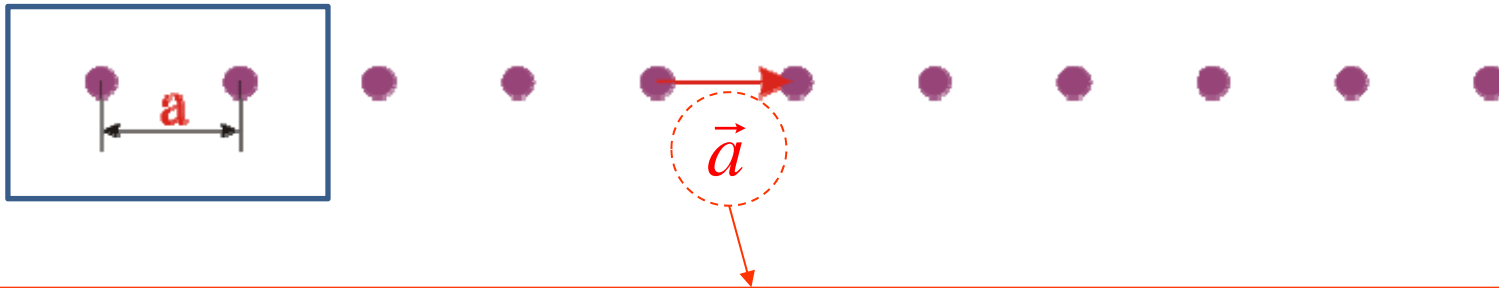
$$\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 \quad (2D)$$

$$\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3 \quad (3D)$$

n_1, n_2, n_3 integer (+, -, or 0)

$a_1, a_2,$ and a_3 not all in same plane (Primitive vector)

1D Lattices



Starting with a point the lattice translation vector (*basis vector*) can generate the lattice

- In 1D there is only one kind of lattice
- This lattice can be described by a single **lattice parameter** (**a**)
- The unit cell for this lattice is a line segment of length **a**

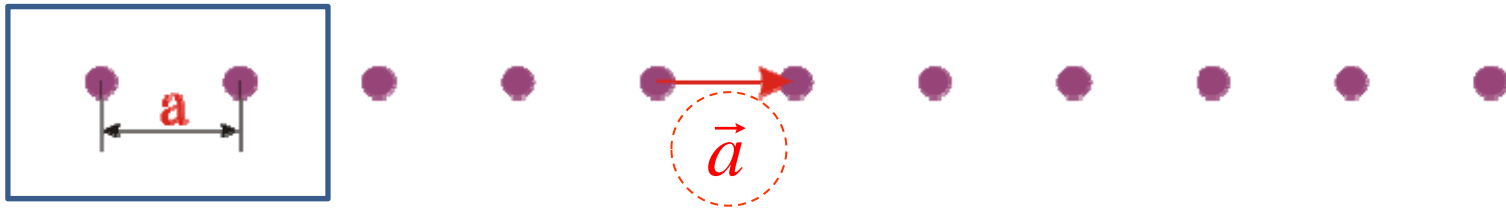
Position vector: $\vec{R} = n_1 \vec{a}_1$

Primitive vector: a_1

primitive cell: ?

Size: a_1

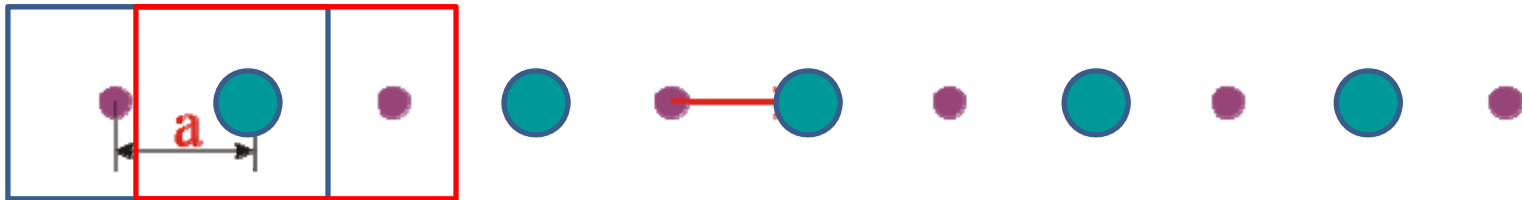
1D Lattices



Position vector: $\vec{R} = n_1 \vec{a}_1$

Primitive vector: a_1

Unit cell: ?

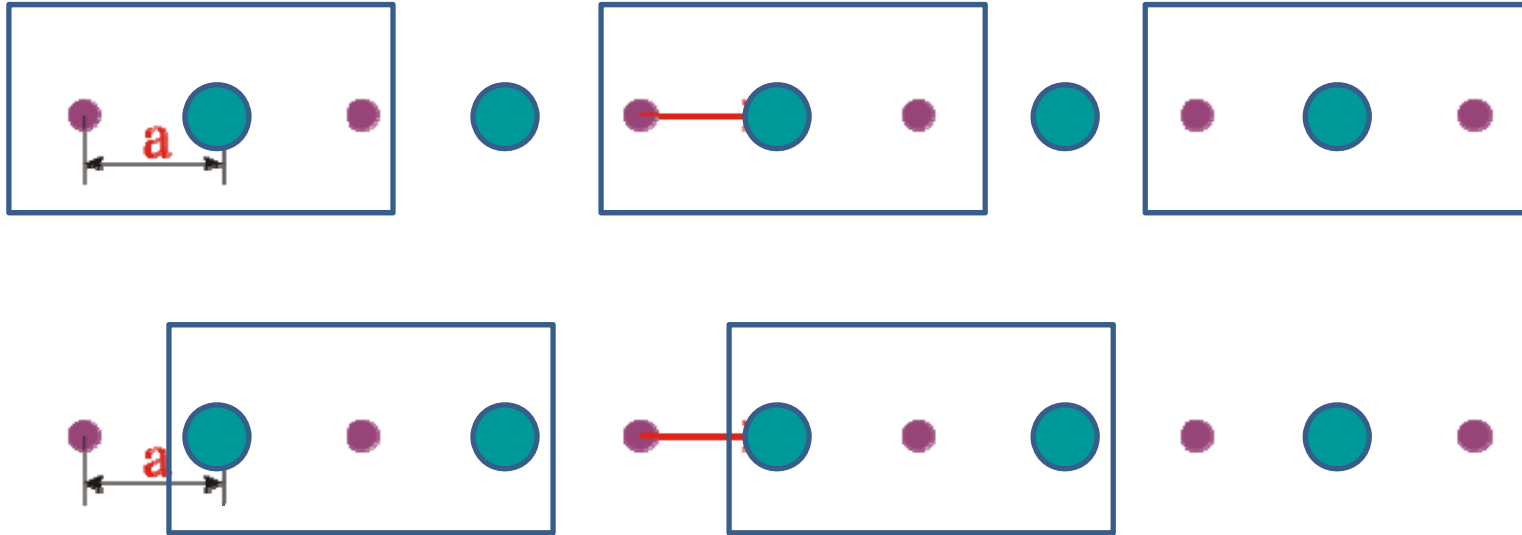


Position vector: ?

Primitive vector: ?

Unit cell: ?

1D Lattices



Position vector: $R = n_1 * (2a)$

Primitive vector: $2a$

primitive cell: ?

2D Lattices

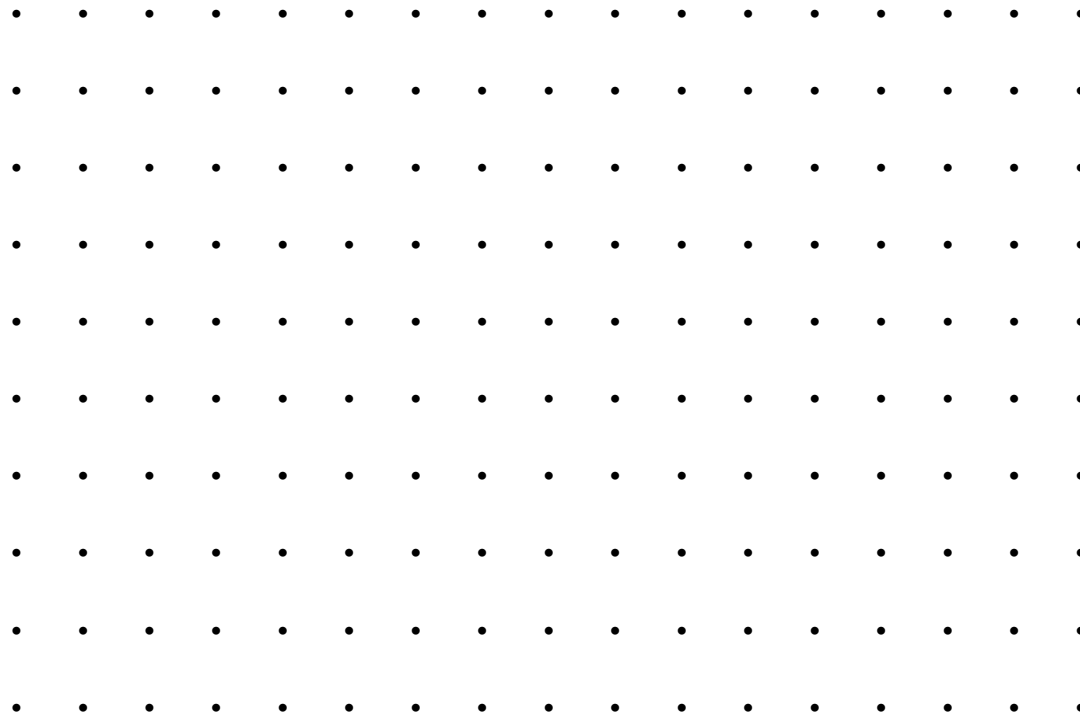
Position vector: $\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2$

Primitive vector: $\mathbf{a}_1, \mathbf{a}_2$

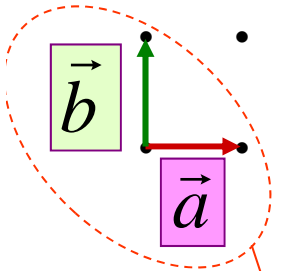
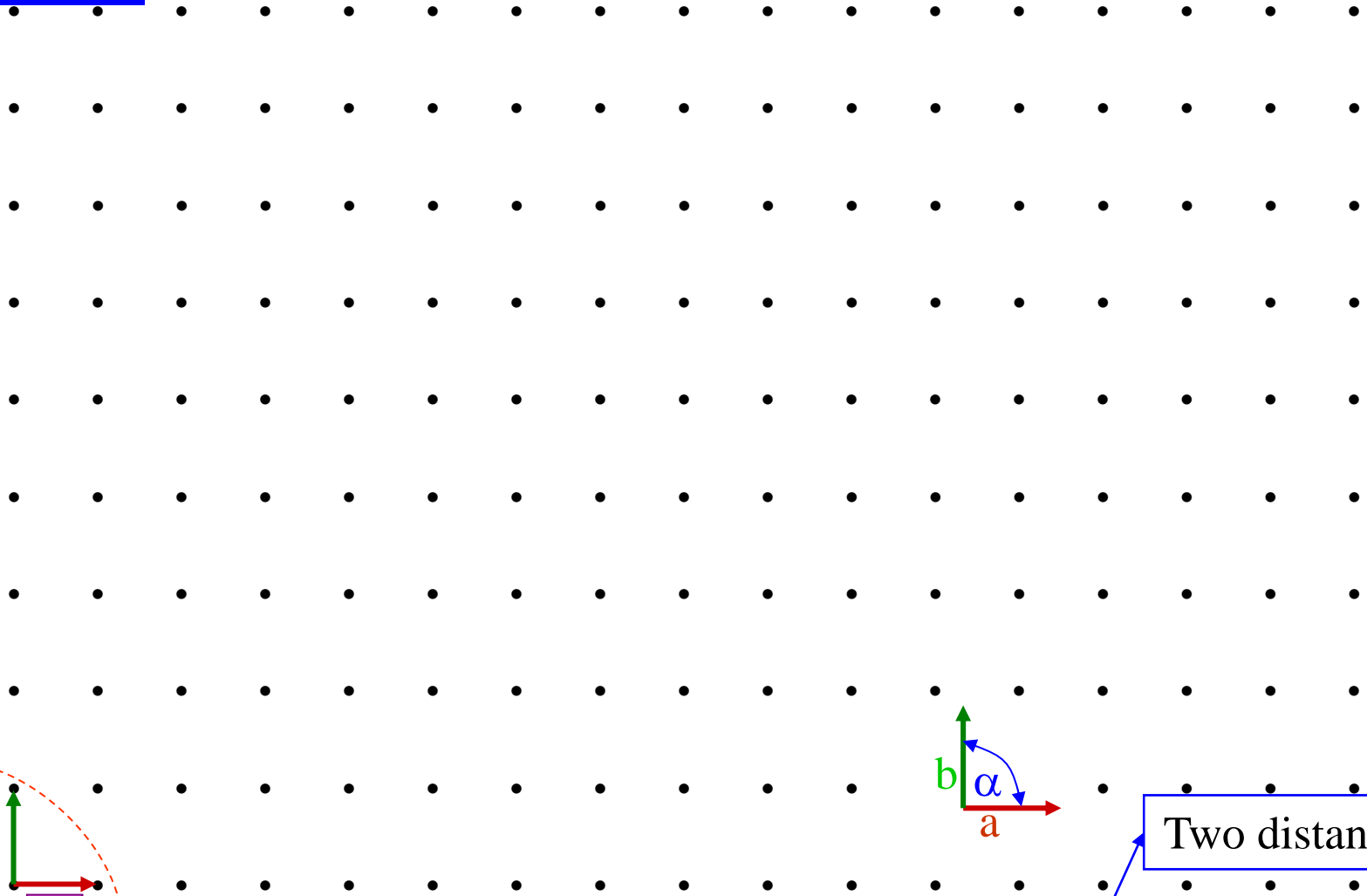
Unit cell:?

Primitive cell:?

Size: $a_1 \times a_2$

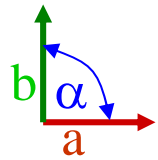


2D Lattices



There are three lattice parameters which describe this lattice

Two basis vectors generate the lattice

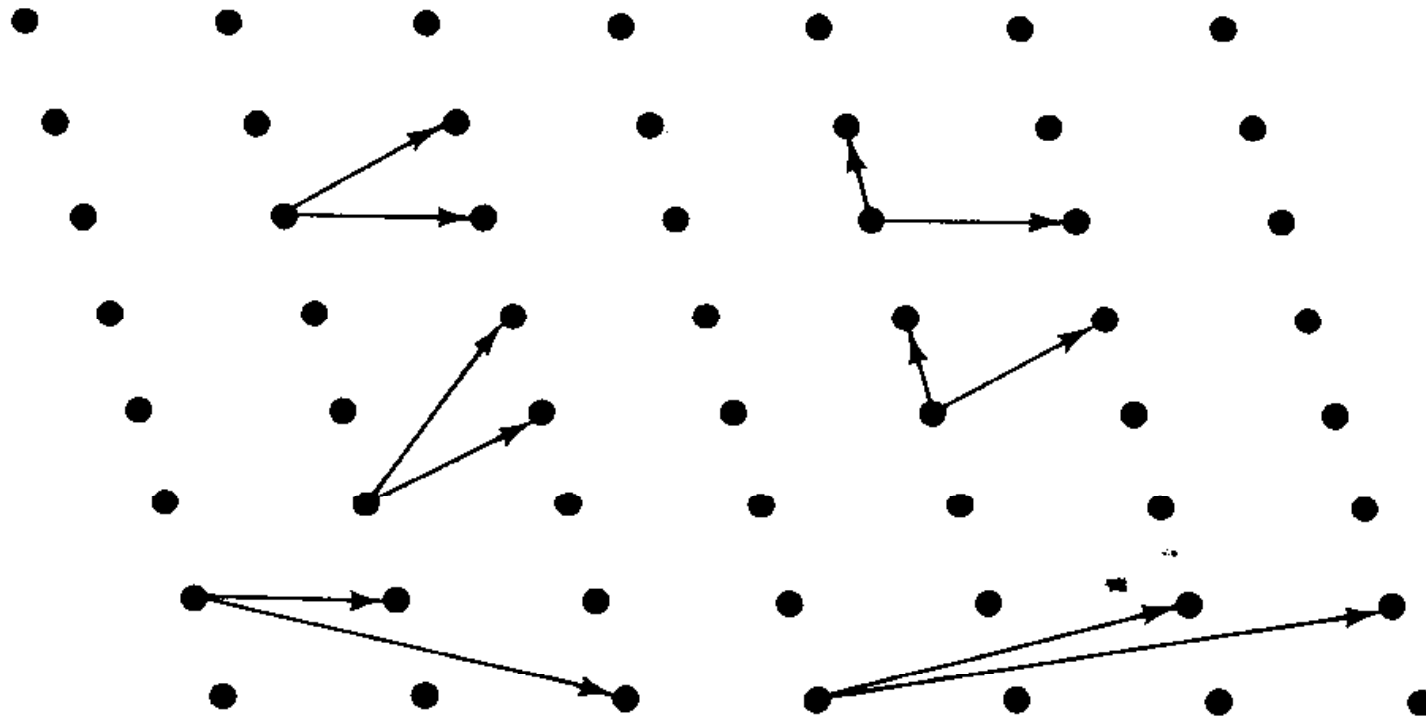


Two distances: a, b

One angle: α

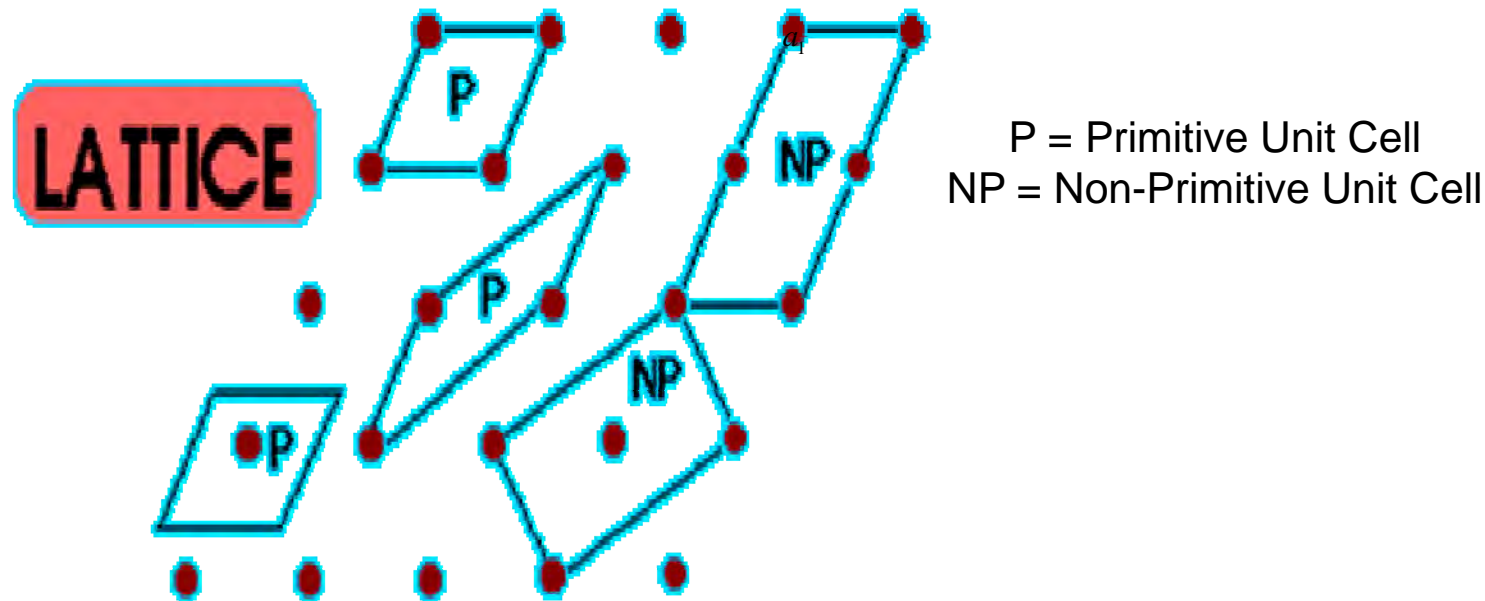
$= 90^\circ$ in the current example

For any given Bravais lattice, the set of primitive vectors is not unique. There are many nonequivalent choices.



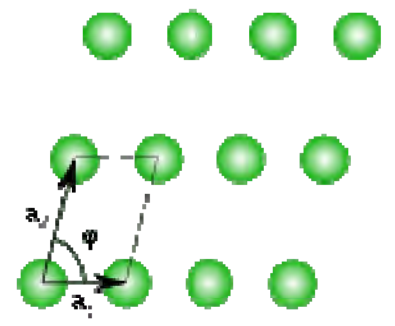
Primitive Unit Cell

- The **primitive unit cell** must have **only one lattice point**.
- There can be **different choices** for lattice vectors , but the volumes of these primitive cells are all the same.



2D Lattices (Five lattices)

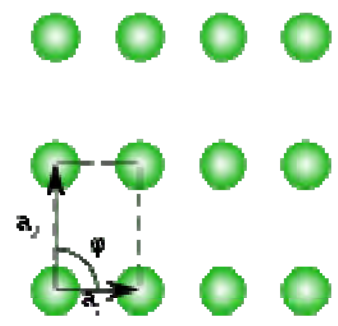
Parallelogram Lattice



$$|a_1| \neq |a_2|, \phi = 90^\circ$$

1

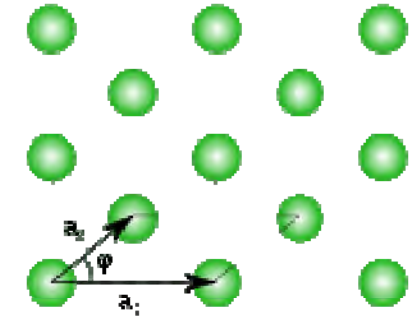
Rectangle Lattice



$$|a_1| \neq |a_2|, \phi = 90^\circ$$

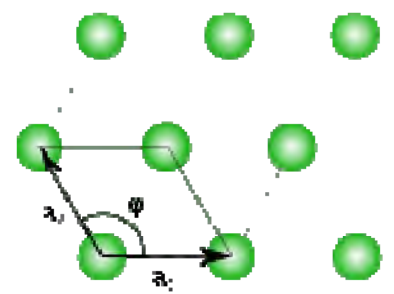
2

Centred Rectangle Lattice



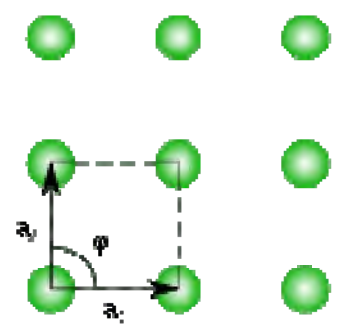
$$|a_1| \neq |a_2|, \phi = 90^\circ$$

3



$$|a_1| = |a_2|, \phi = 120^\circ$$

120° Rhombus Lattice

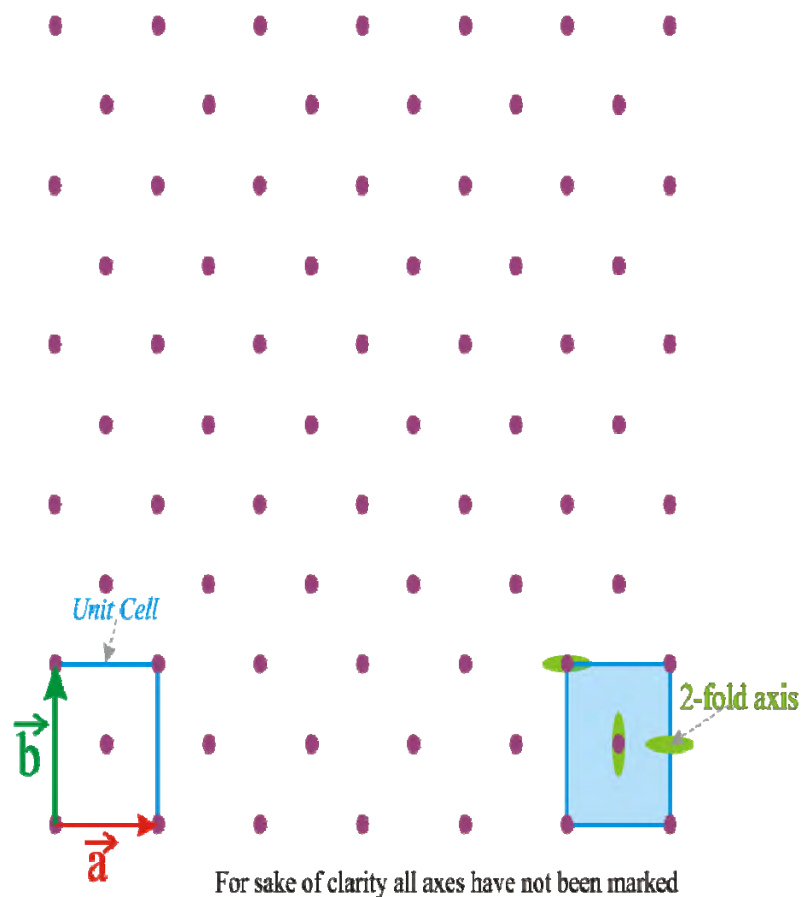


$$|a_1| = |a_2|, \phi = 90^\circ$$

5

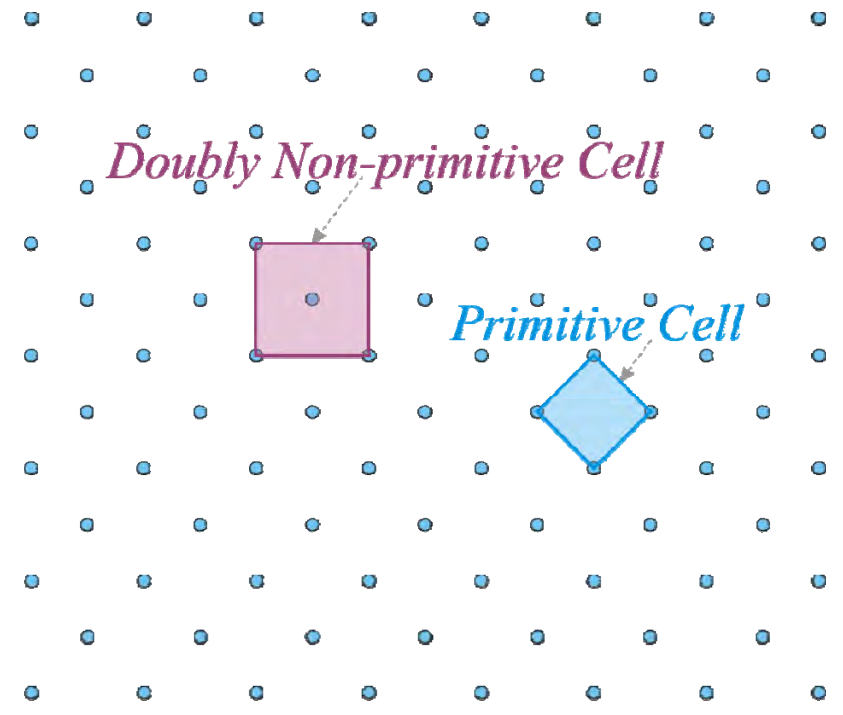
Square Lattice

Centred Rectangle Lattice



Lattice parameters: $a, b, \alpha - 90^\circ$

Centred cubic Lattice?



Summary of 2D lattices

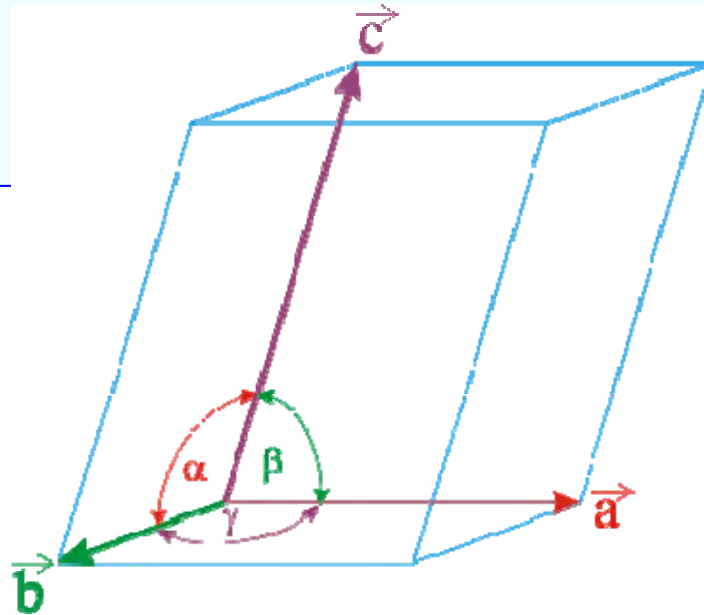
Lattice	Symmetry	Shape of UC	Lattice Parameters
1. Square	4mm	1. Square	($a = b$, $\alpha = 90^\circ$)
2. Rectangle	2mm	2. Rectangle	($a \neq b$, $\alpha = 90^\circ$)
3. Centred Rectangle	2mm	"	($a \neq b$, $\alpha = 90^\circ$)
4. 120° Rhombus	6mm	3. 120° Rhombus	($a = b$, $\alpha = 120^\circ$)
5. Parallelogram	2	4. Parallelogram	($a \neq b$, α general value)

Lattice	Simple	Centred
Square	✓	✗
Rectangle	✓	✓
120° Rhombus	✓	✗
Parallelogram	✓	✗

Every lattice that you can construct is present somewhere in the list
 → *the issue is where to put them!*
Shows the equivalence

3D Lattices

- ❑ 3D lattices can be generated with three basis vectors
 - ❑ They are infinite in three dimensions
 - ❑ 3 basis vectors generate a 3D lattice
- ❑ The unit cell of a general 3D lattice is described by 6 numbers (in special cases all these numbers need not be independent) → **6 lattice parameters**



3D Lattices (14)

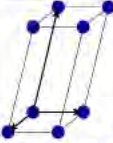
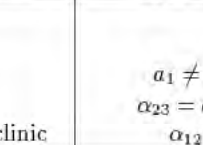
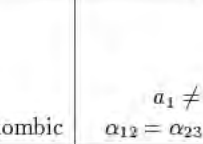
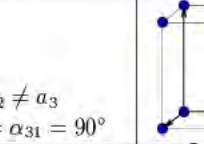
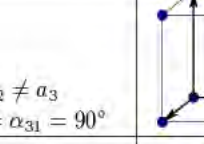
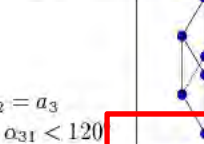
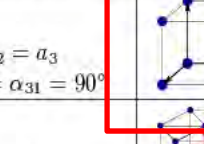
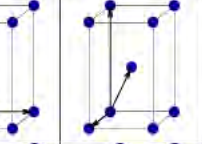
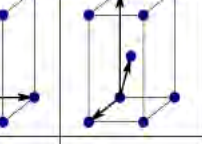
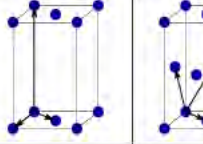


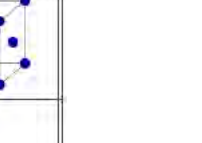

Bravais lattice	Parameters	Simple (P)	Volume centered (I)	Base centered (C)	Face centered (F)
Triclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{12} \neq \alpha_{23} \neq \alpha_{31}$				
Monoclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{23} = \alpha_{31} = 90^\circ$ $\alpha_{12} \neq 90^\circ$				
Orthorhombic	$a_1 \neq a_2 \neq a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90^\circ$				
Tetragonal	$a_1 = a_2 \neq a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90^\circ$				
Trigonal	$a_1 = a_2 = a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} < 120^\circ$				
Cubic	$a_1 = a_2 = a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90^\circ$				
Hexagonal	$a_1 = a_2 \neq a_3$ $\alpha_{12} = 120^\circ$ $\alpha_{23} = \alpha_{31} = 90^\circ$				

Table 1.1: Bravais lattices in three-dimensions.

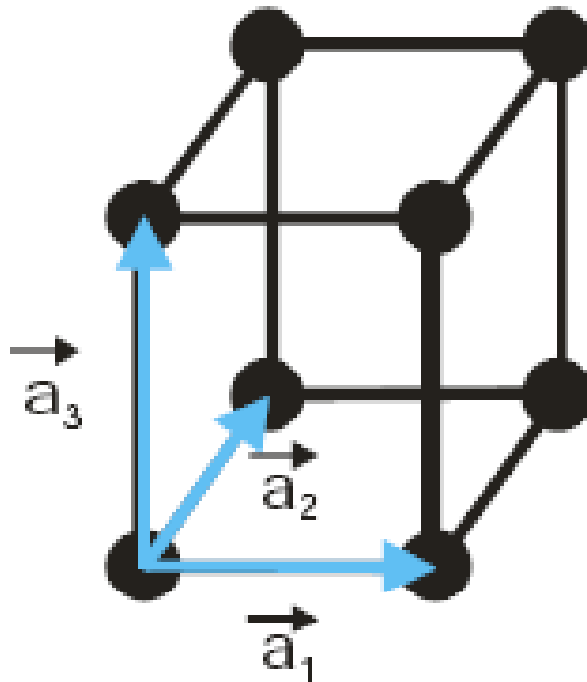
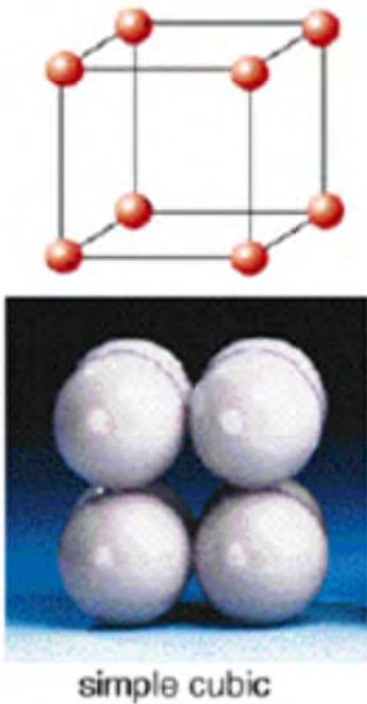
Cubic(P)

Position vector: $\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$

Primitive vector: a_1, a_2, a_3

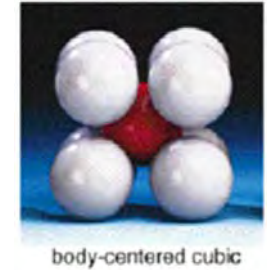
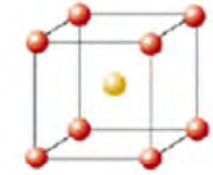
Primitive cell: ?

Size: $a_1 \cdot (a_2 \times a_3)$

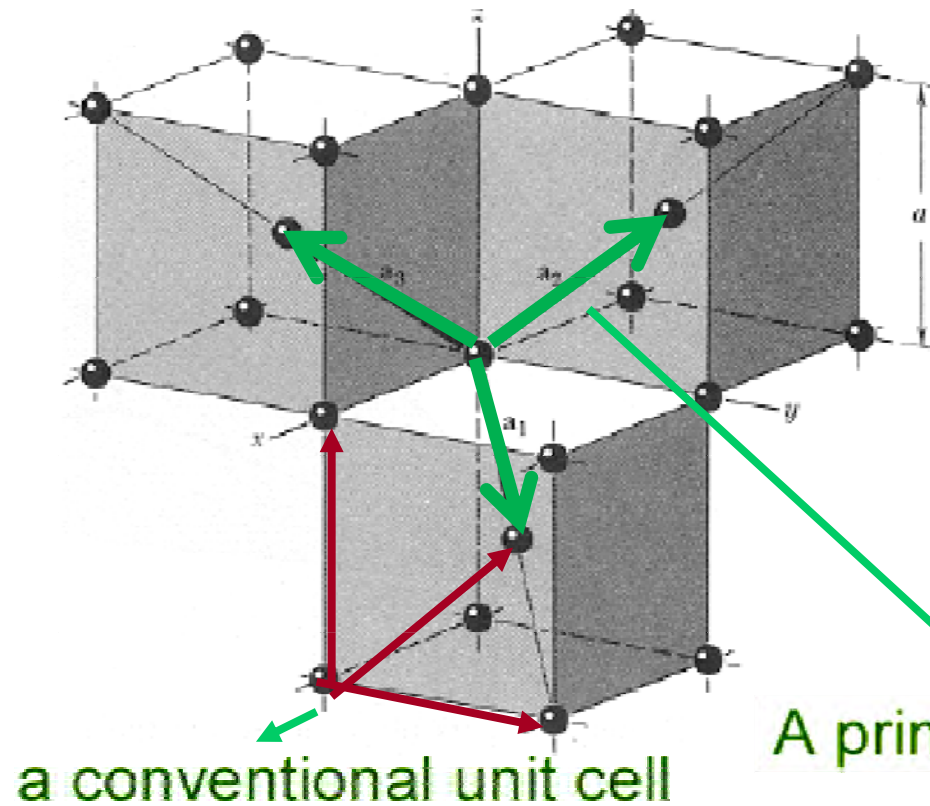


$$V = a^3$$

Cubic(I)



Primitive and conventional cells



Primitive Translation Vectors:

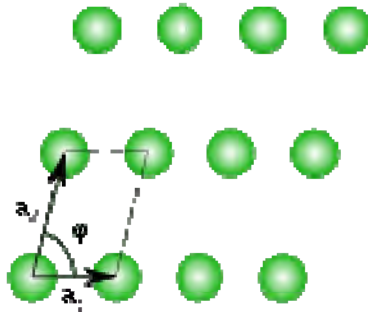
$$\vec{a}_1 = \frac{1}{2}(\hat{x} - \hat{y} - \hat{z})$$

$$\vec{a}_2 = \frac{1}{2}(-\hat{x} + \hat{y} + \hat{z})$$

$$\vec{a}_3 = \frac{1}{2}(\hat{x} + \hat{y} - \hat{z})$$

2D (5 lattice)

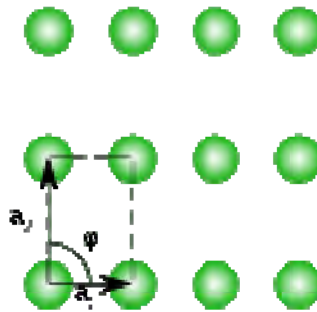
Parallelogram Lattice



$$|a_1| \neq |a_2|, \varphi = 90^\circ$$

1

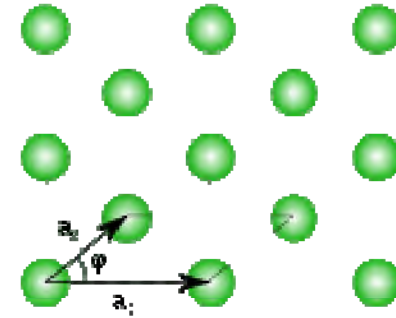
Rectangle Lattice



$$|a_1| \neq |a_2|, \varphi = 90^\circ$$

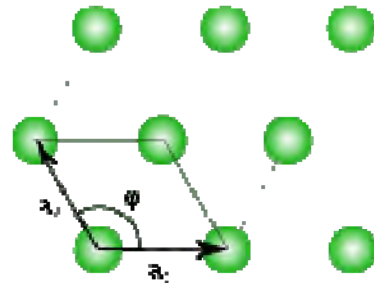
2

Centred Rectangle Lattice



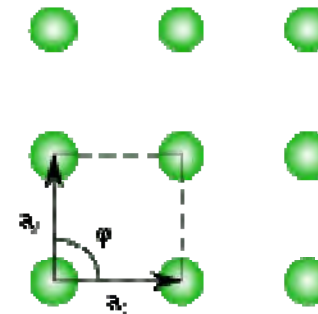
$$|a_1| \neq |a_2|, \varphi = 90^\circ$$

3



$$|a_1| = |a_2|, \varphi = 120^\circ$$

120° Rhombus Lattice



$$|a_1| = |a_2|, \varphi = 90^\circ$$

5

Square Lattice

3D Lattices (14)

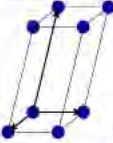
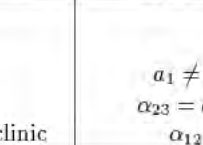
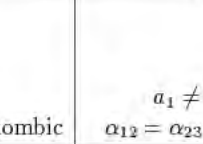
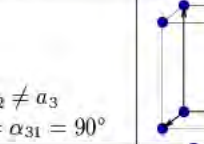
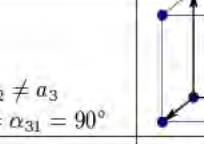
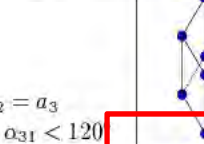
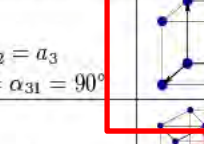
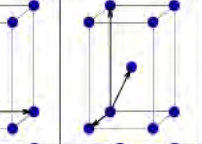
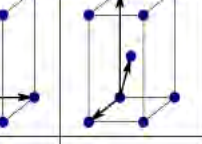
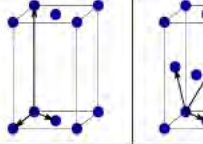


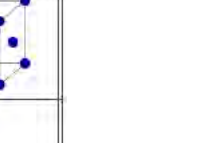

Bravais lattice	Parameters	Simple (P)	Volume centered (I)	Base centered (C)	Face centered (F)
Triclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{12} \neq \alpha_{23} \neq \alpha_{31}$				
Monoclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{23} = \alpha_{31} = 90^\circ$ $\alpha_{12} \neq 90^\circ$				
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Table 1.1: Bravais lattices in three-dimensions.

Bravais Lattice

1, An array of points such that every point has *identical surroundings*

2, *primitive lattice: (a minimum-volume unit cell)*

3, *position vector:*

$$\vec{R} = n_1 \vec{a}_1 \quad (1D)$$

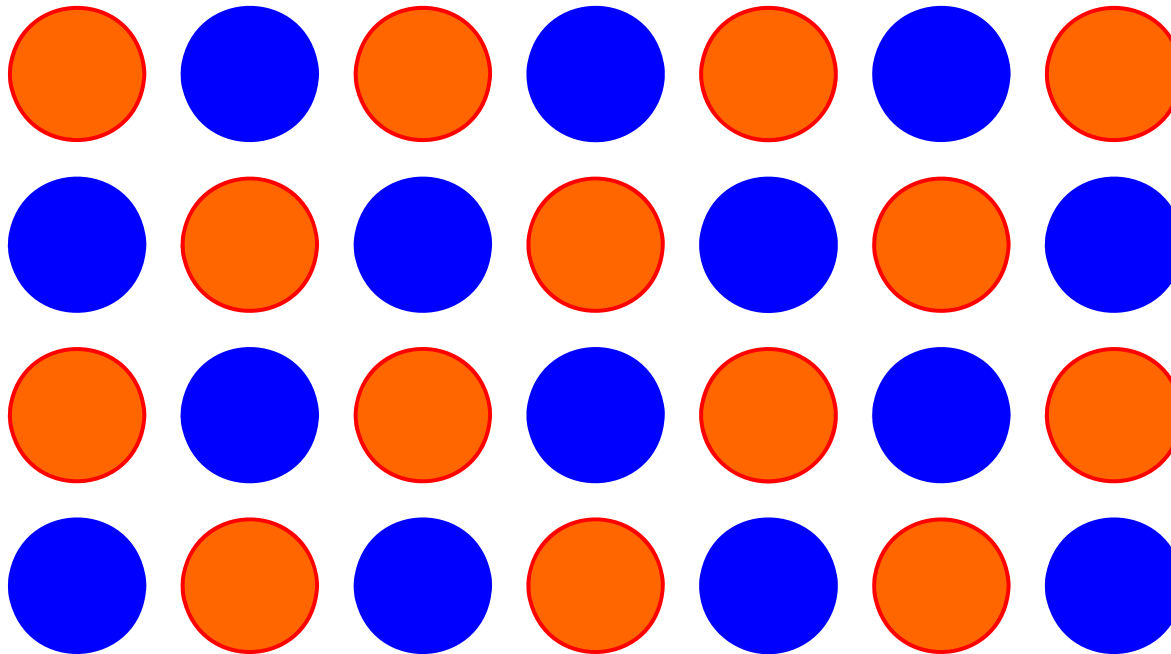
$$\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 \quad (2D)$$

$$\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3 \quad (3D)$$

n_1, n_2, n_3 integer (+, -, or 0)

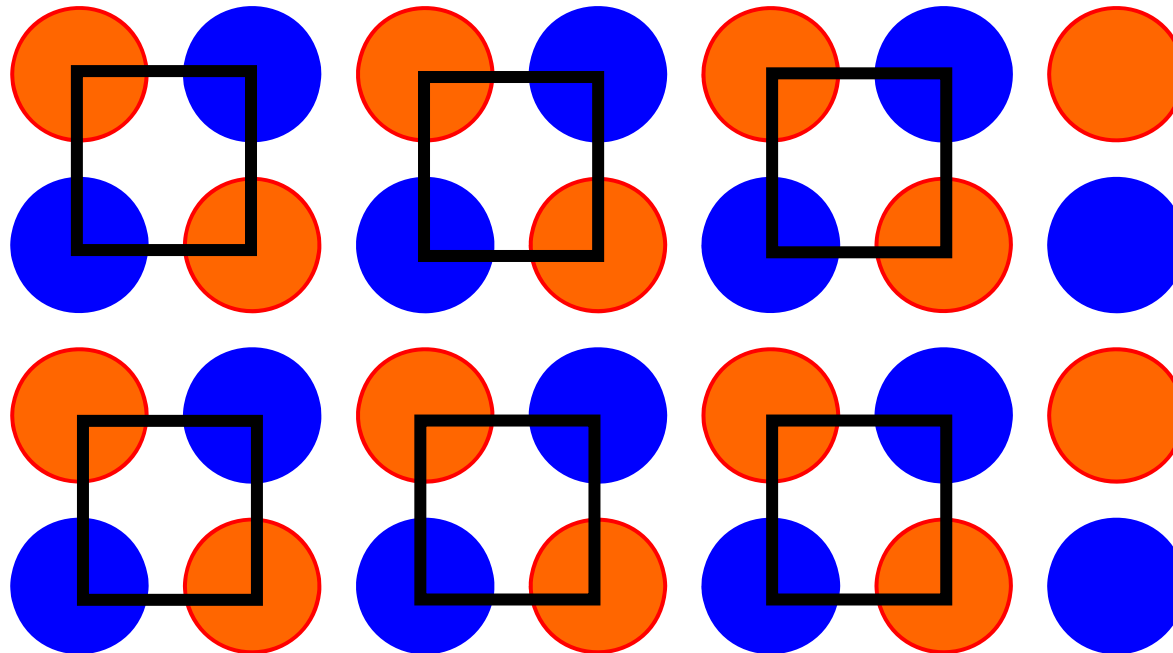
$a_1, a_2,$ and a_3 not all in same plane (Primitive vector)

2D Unit Cell example - (NaCl)



We define lattice points ; these are points with *identical environments*

This is NOT a unit cell even though they are all the same
- empty space is not allowed!



In 2D, this IS a unit cell

