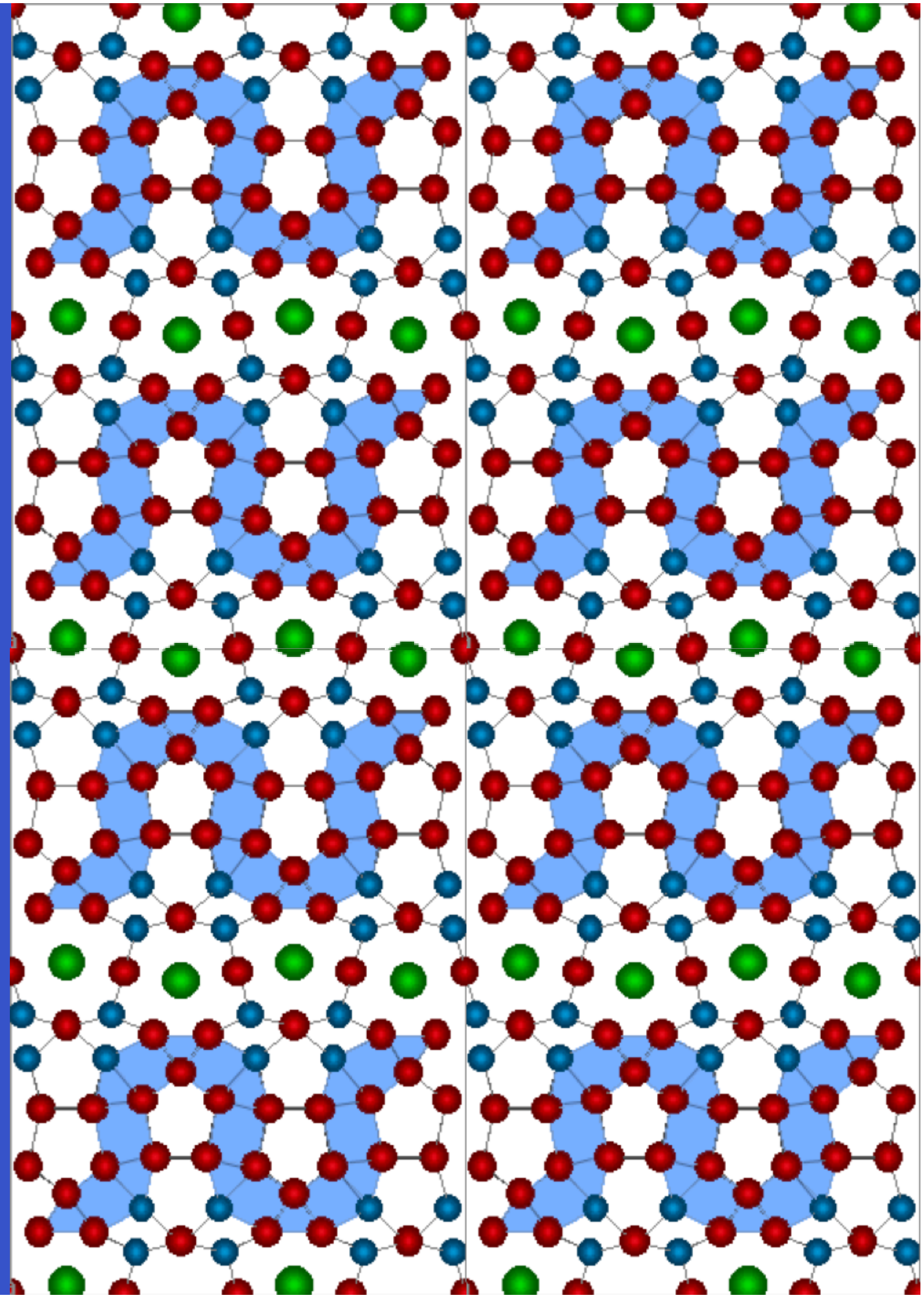
crystallography

(晶体学)



Most materials we use are crystalline, partially crystalline, or can be made crystalline or partially crystalline

Crystalline means atom arrangement is periodic (周期性的) - repeats throughout space

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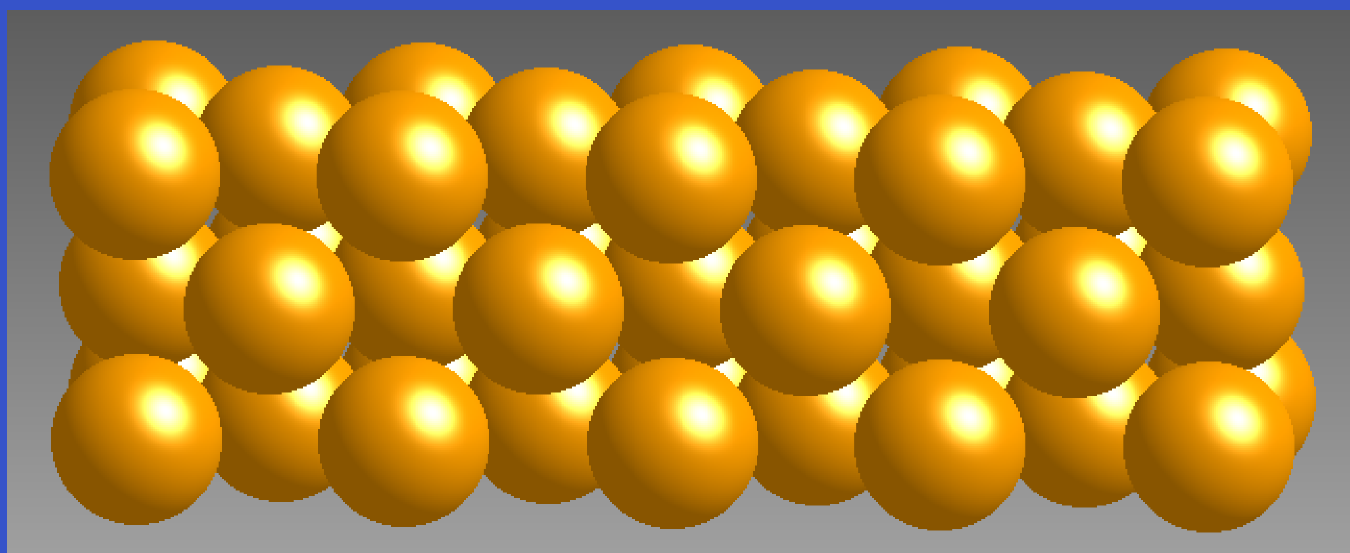

metals

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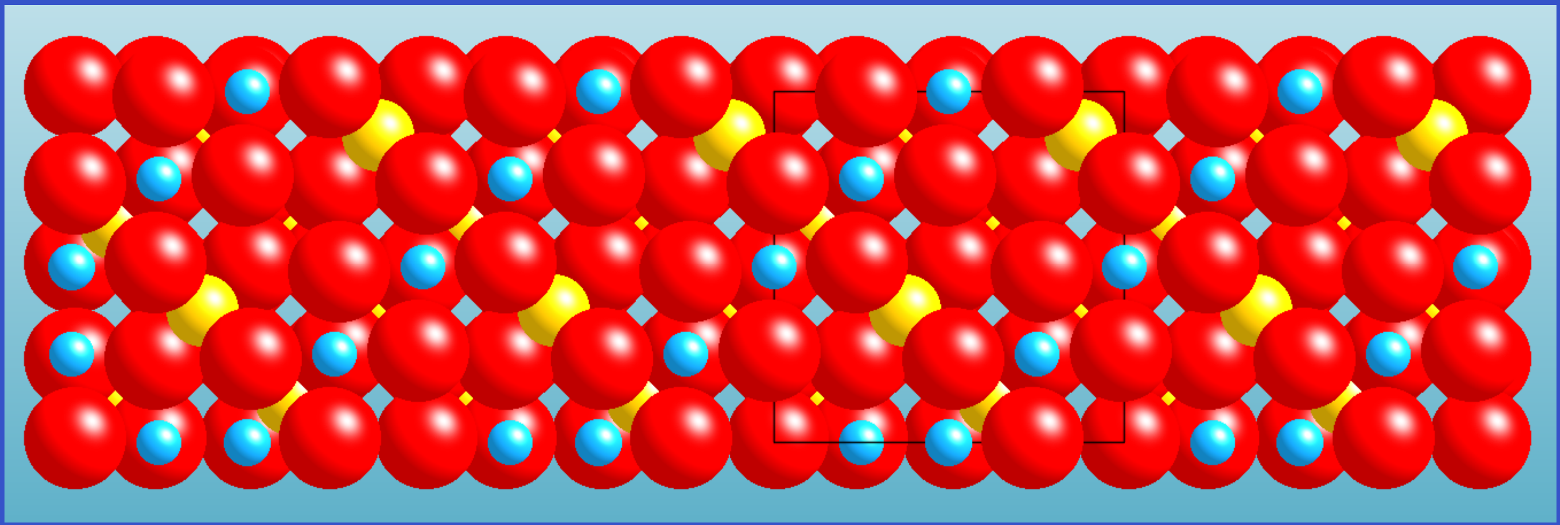

spinels (ferrites - 铁电的)

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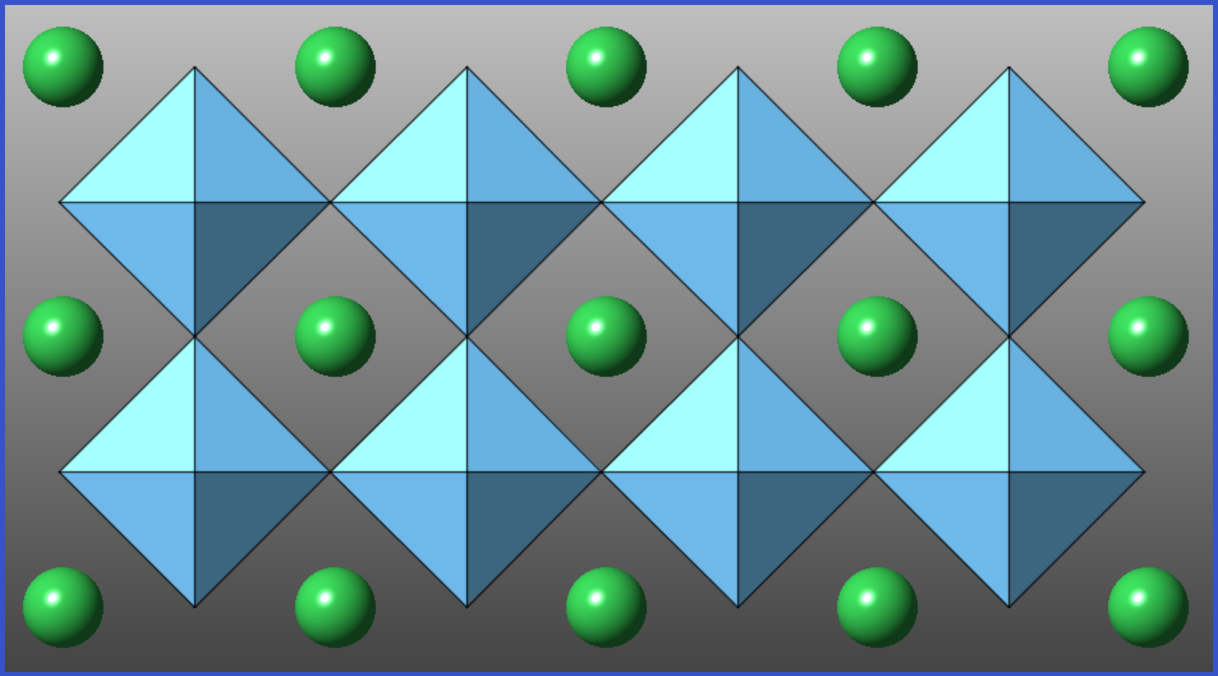

$BaTiO_3$
(钡钛氧$_3$)

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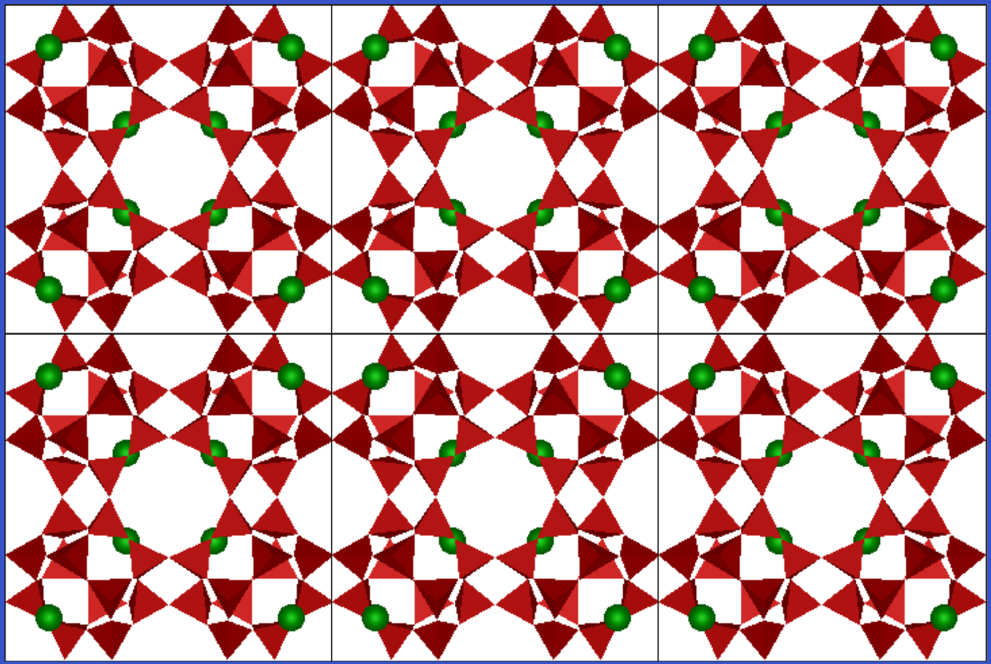

zeolite (沸石)

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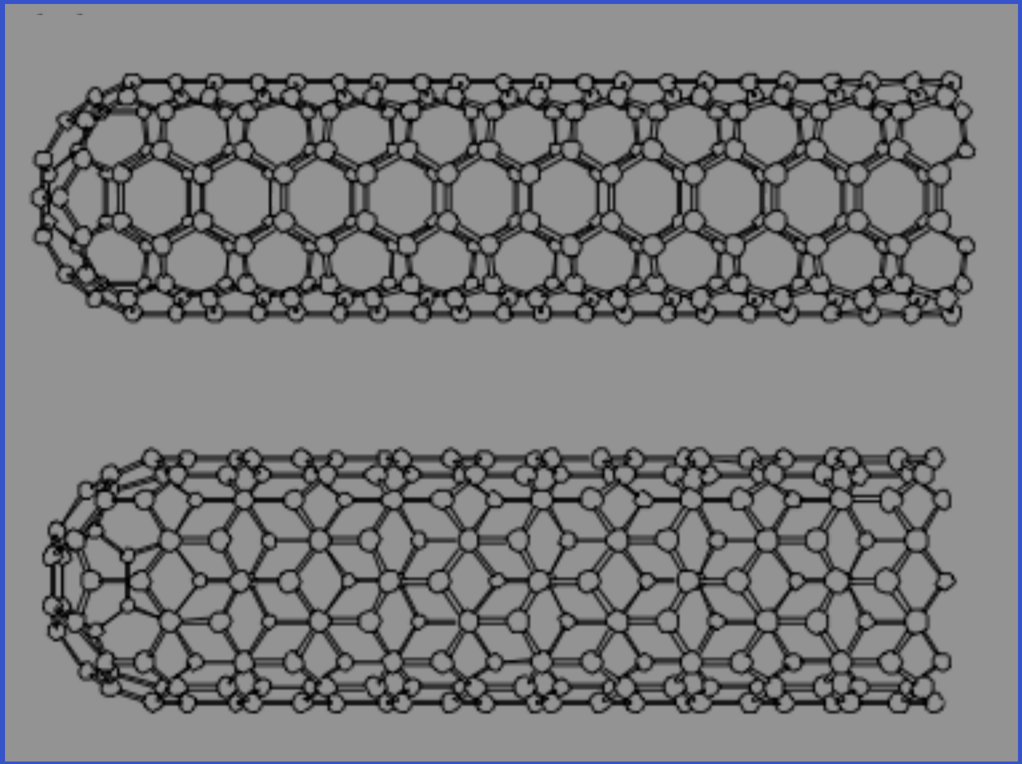
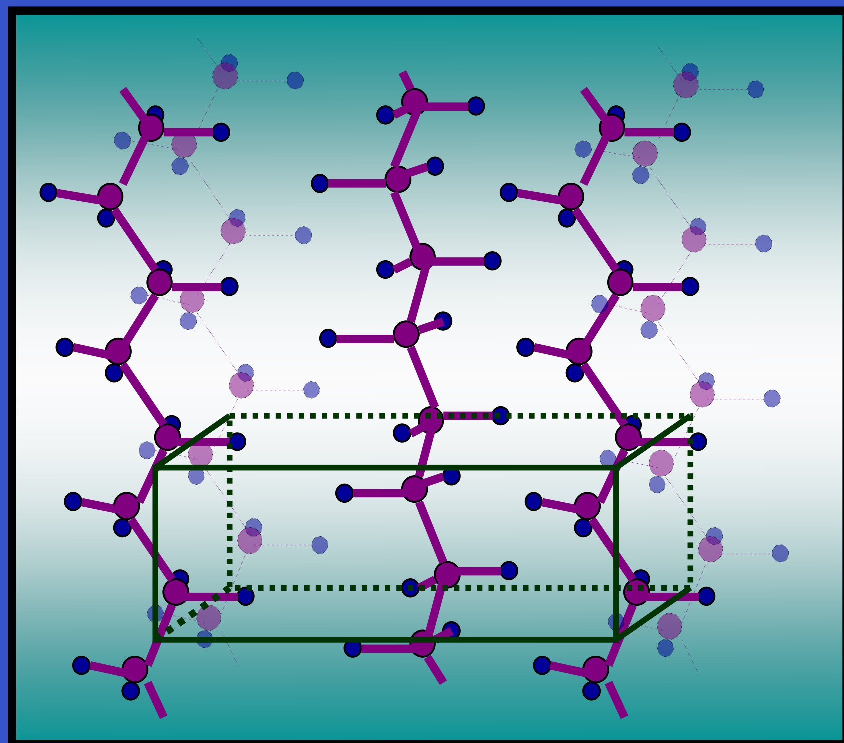


carbon nanotubes (纳米管) (CNTs)

Most materials we use are crystalline, partially crystalline, or can be made crystalline or partially crystalline



polyethylene (聚乙烯) polymer

This type of structure is called

crystal structure (晶体结构)

In crystals, atom groups (unit cells) repeated to form a solid material

The study of this repetition in crystals is called crystallography

Repetition = symmetry (对称性)

Types of repetition:

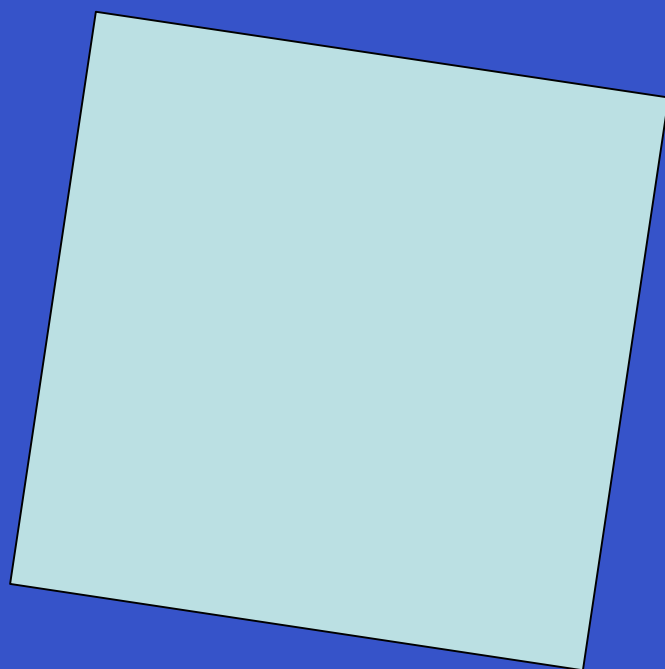
rotation (旋转)
translation (平移)

Rotation

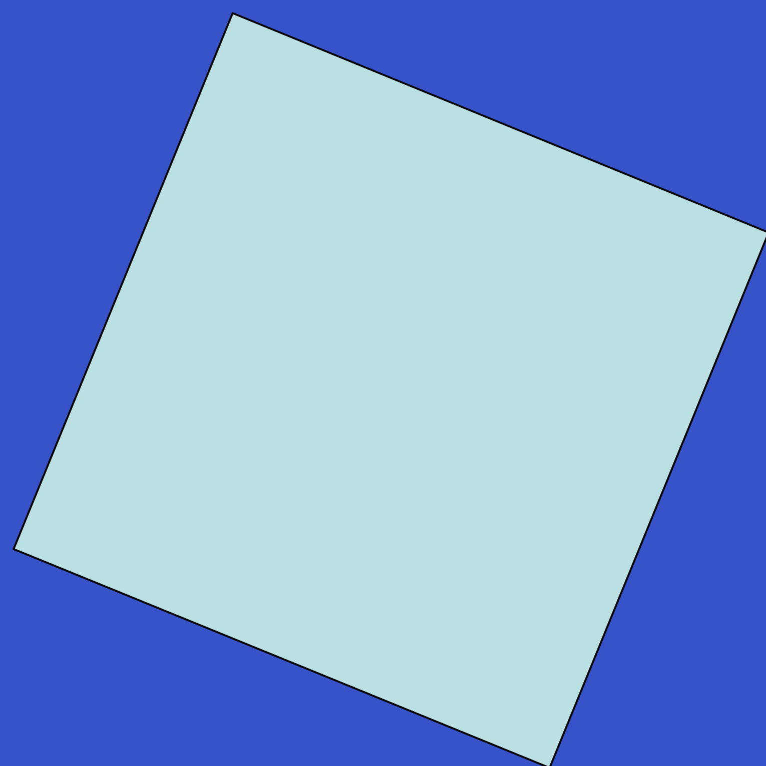
What is rotational symmetry?

Imagine this object will be rotated (maybe)

Imagine this object will be rotated (maybe)



Imagine this object will be rotated (maybe)



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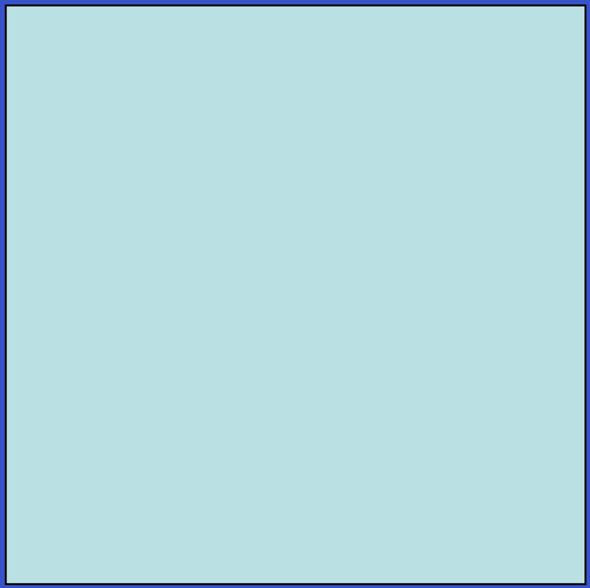
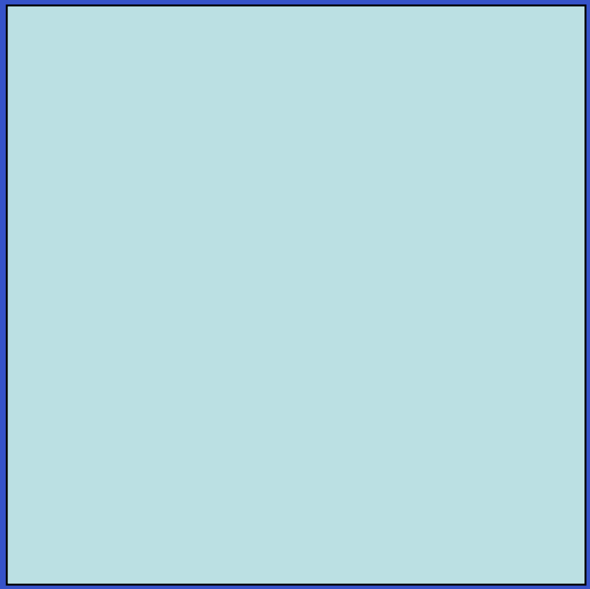


Was it?

The object is obviously symmetric…it has symmetry



The object is obviously symmetric…it has symmetry

Can be rotated 90° w/o detection

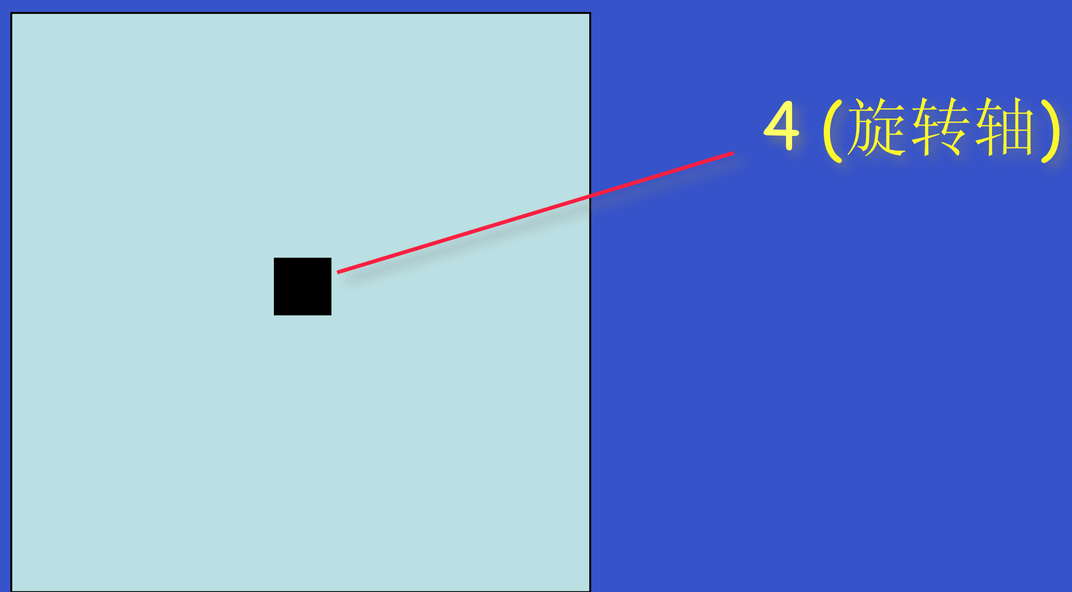
…………so symmetry is really

doing nothing

Symmetry is doing nothing - or at least doing something so that it looks like nothing was done!

What kind of symmetry does this object have?

What kind of symmetry does this object have?



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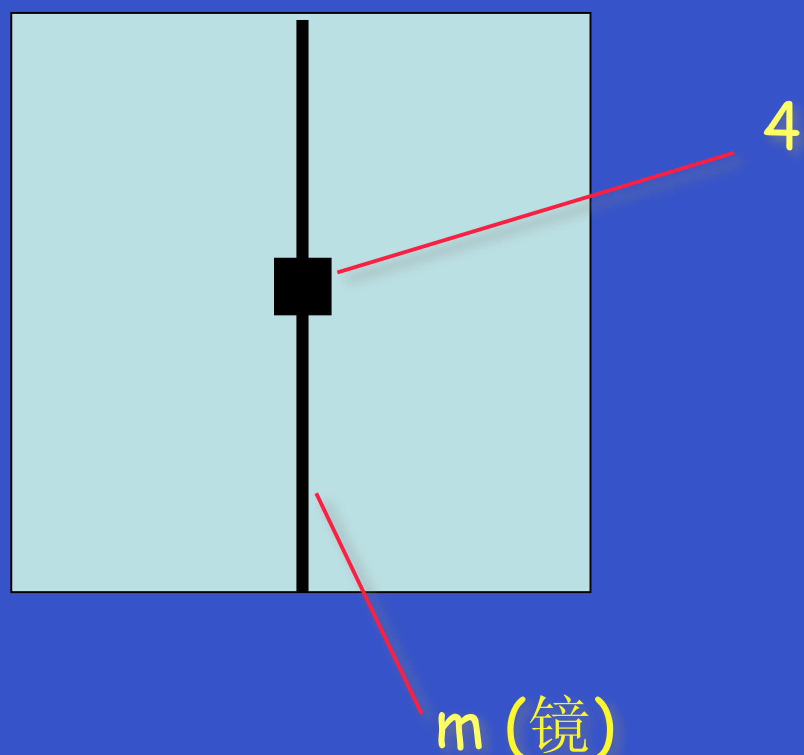

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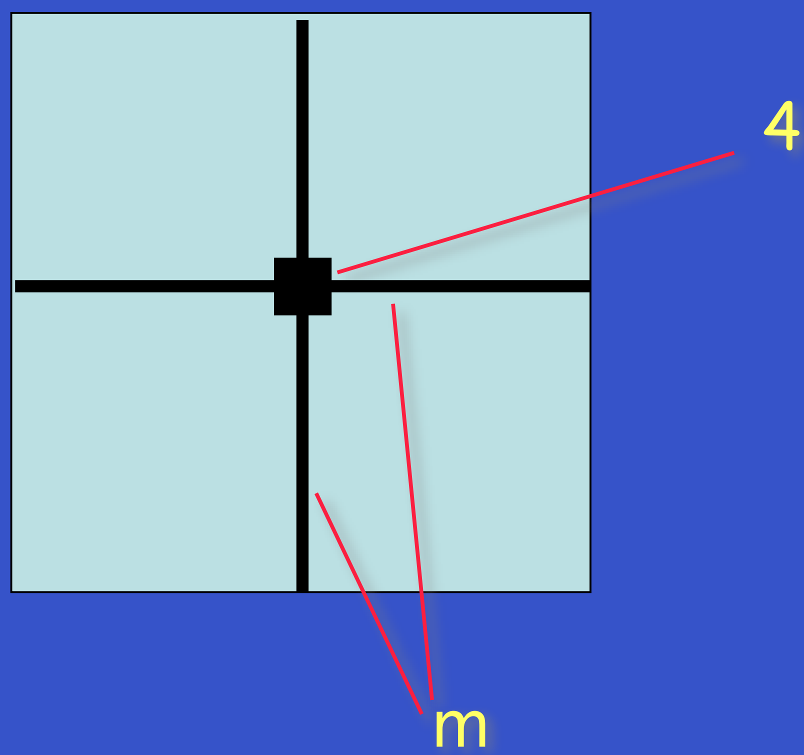

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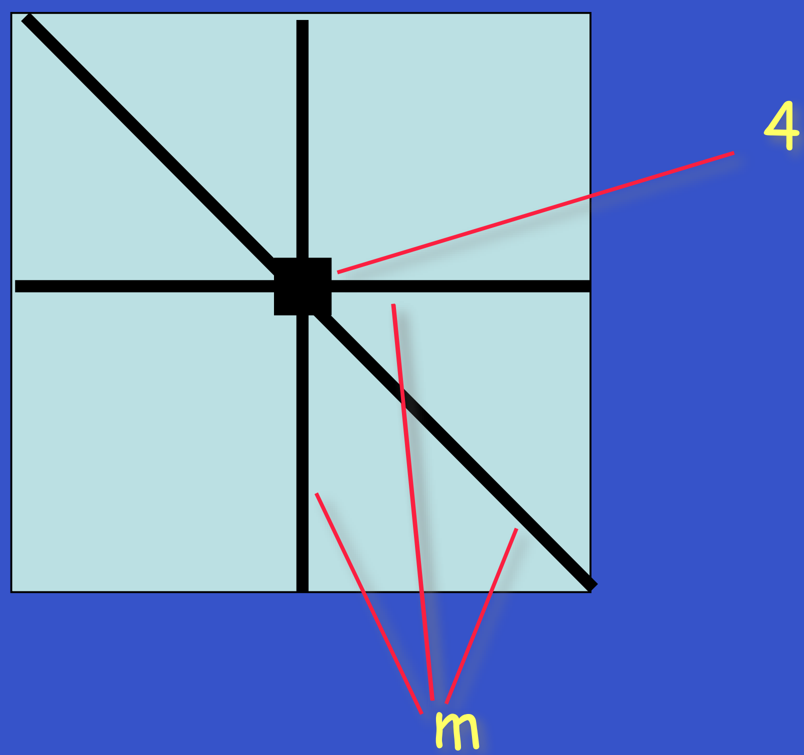

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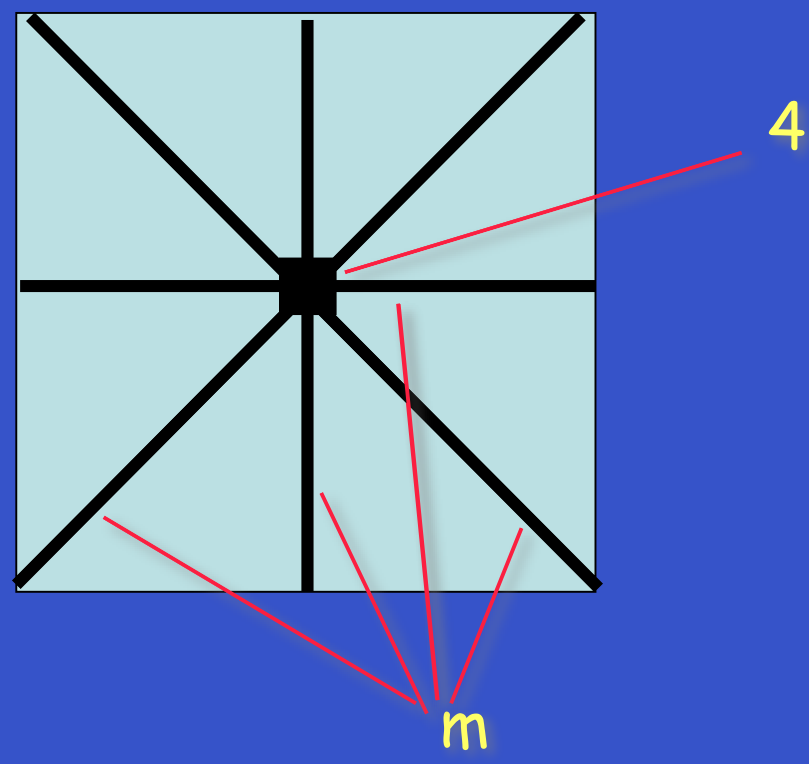
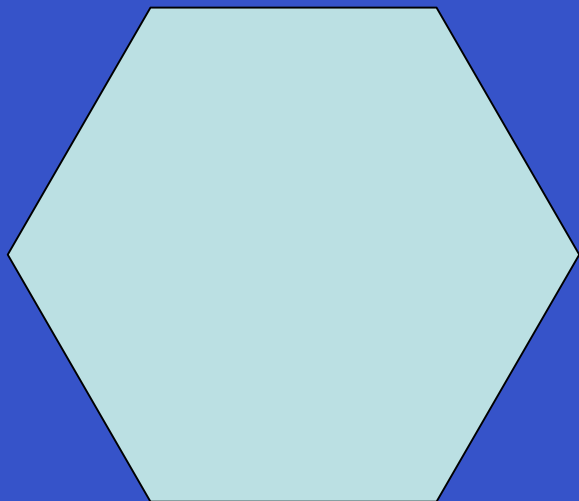
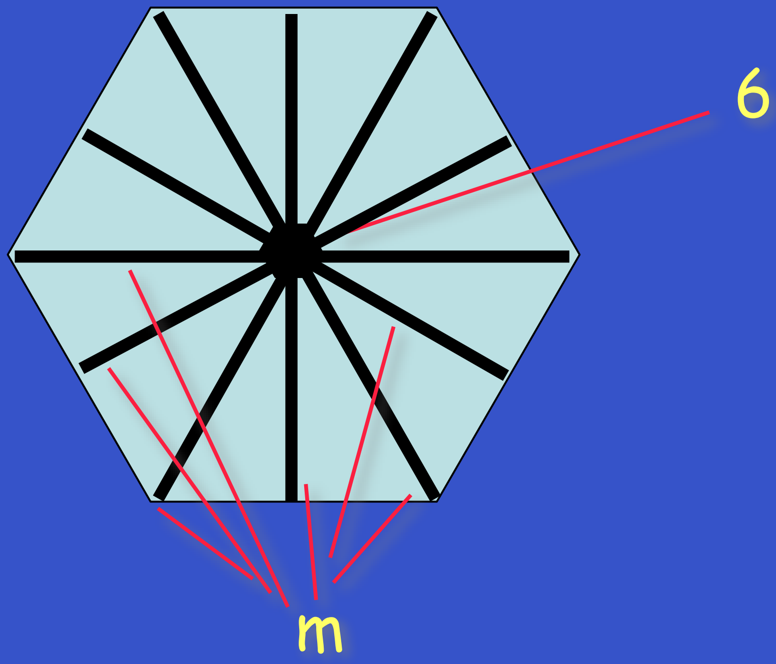


4mm
(点群)

Another example:



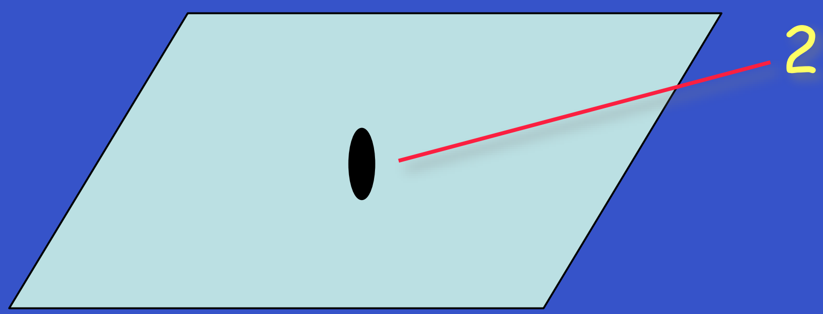
Another example:



6mm

And another:

And another:



2

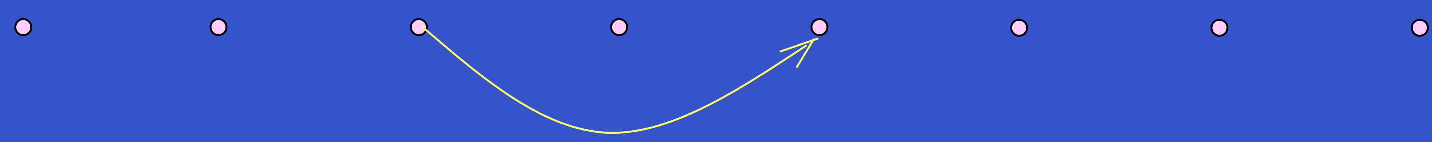
What about translation?

Same as rotation

What about translation?

Same as rotation

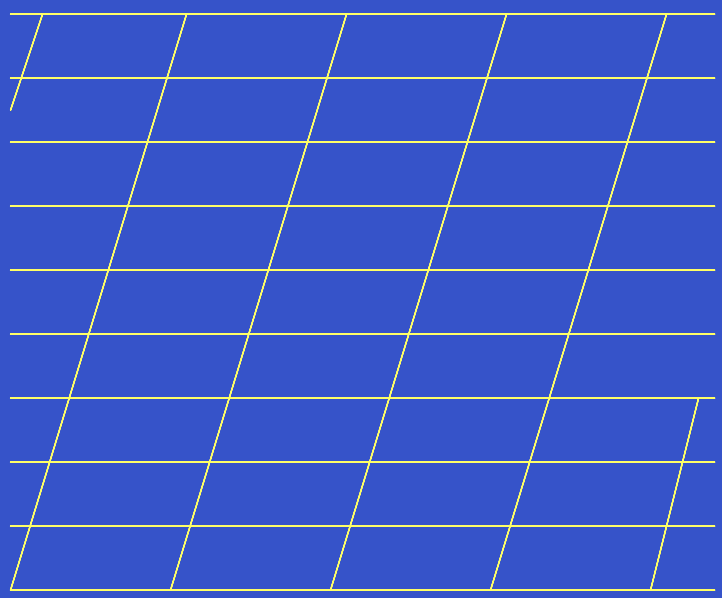
Ex: one dimensional array of points



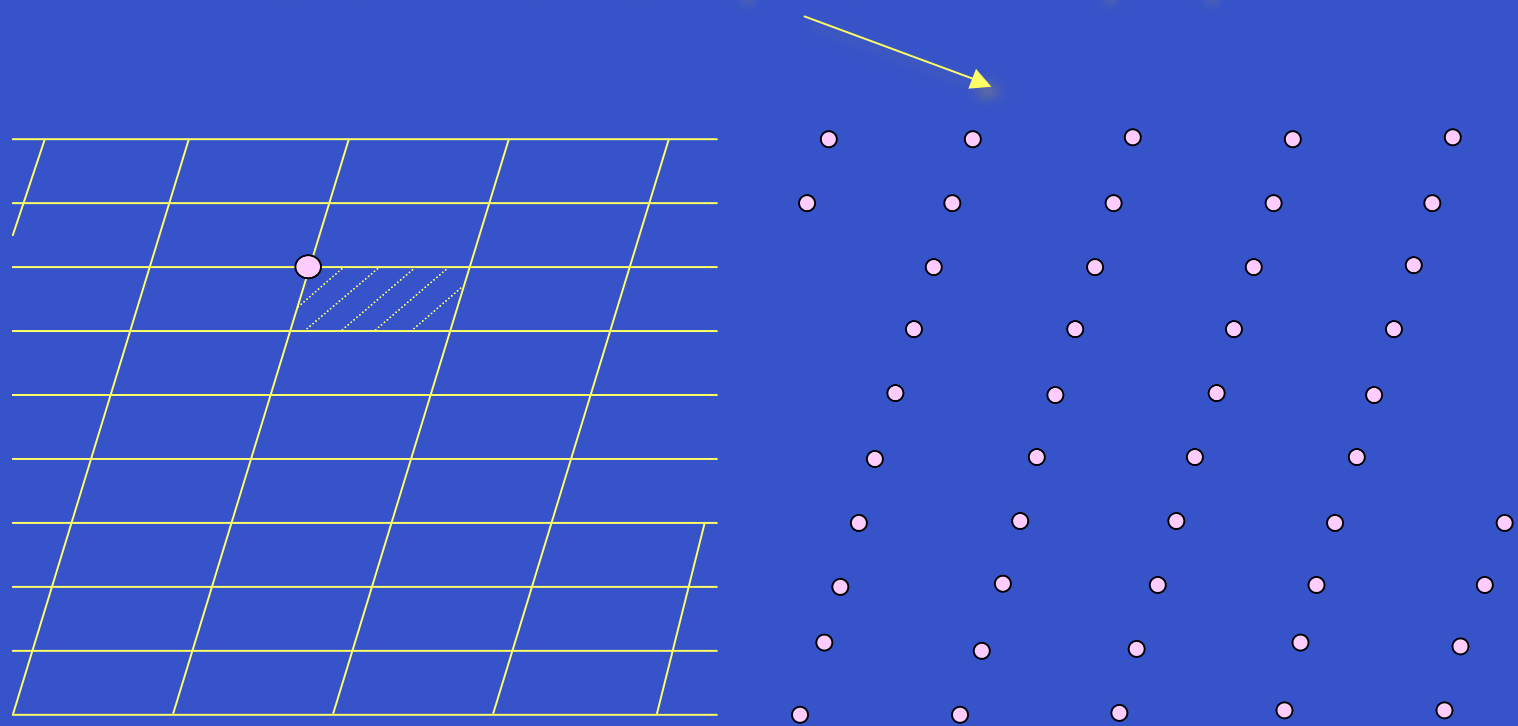
Translations are restricted to only certain values to get symmetry (periodicity)

2D translations

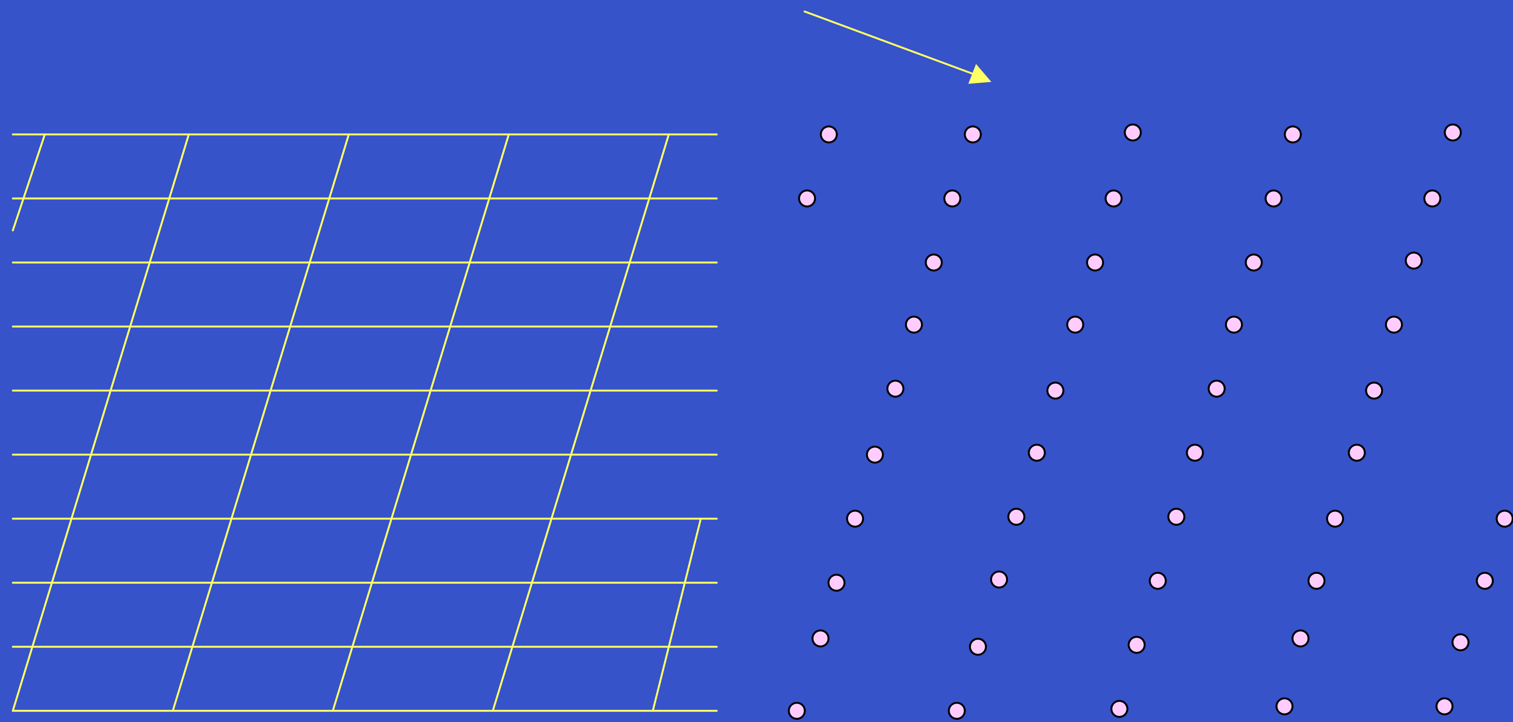
Lots of common examples



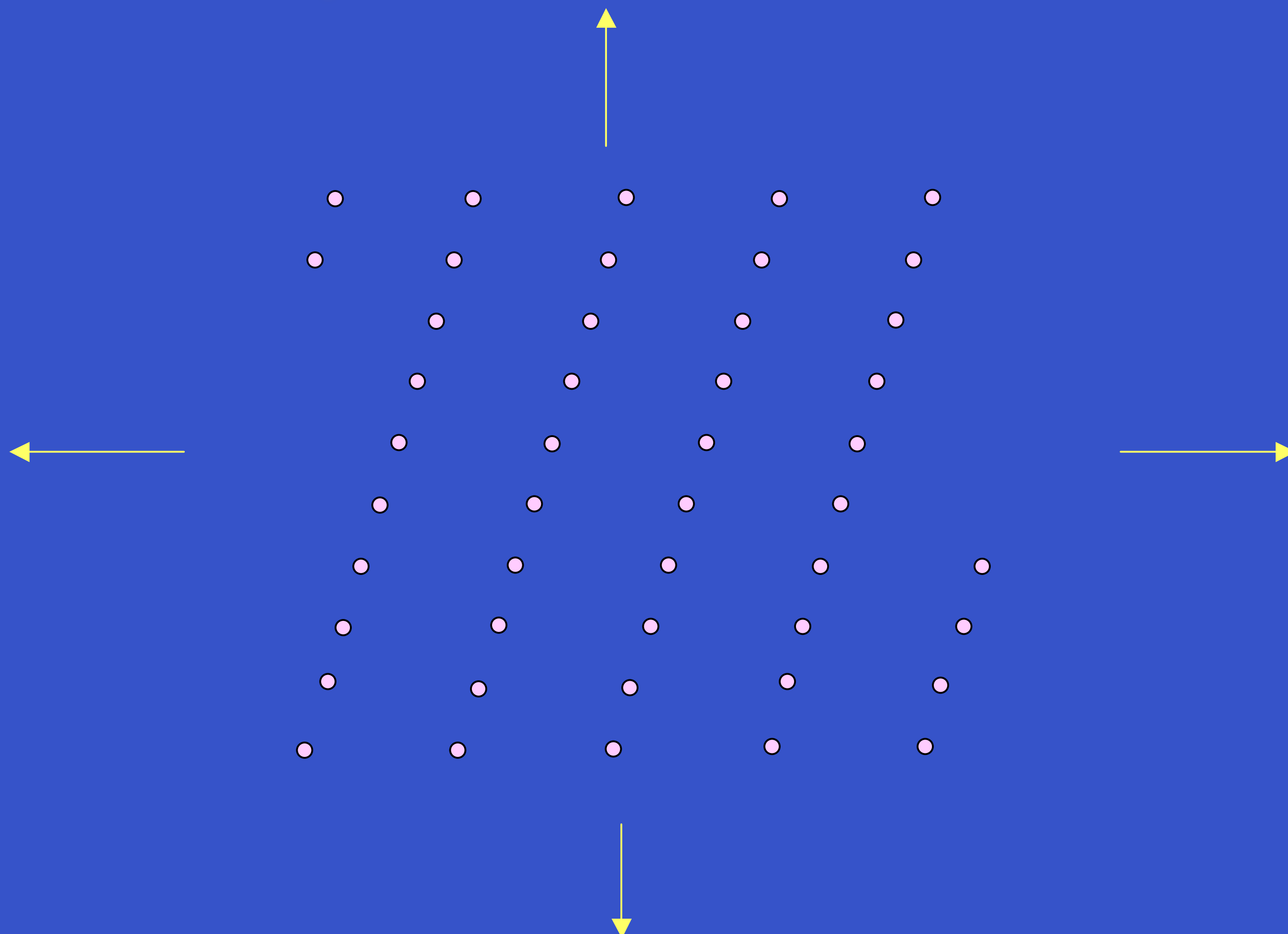
Each block is represented by a point



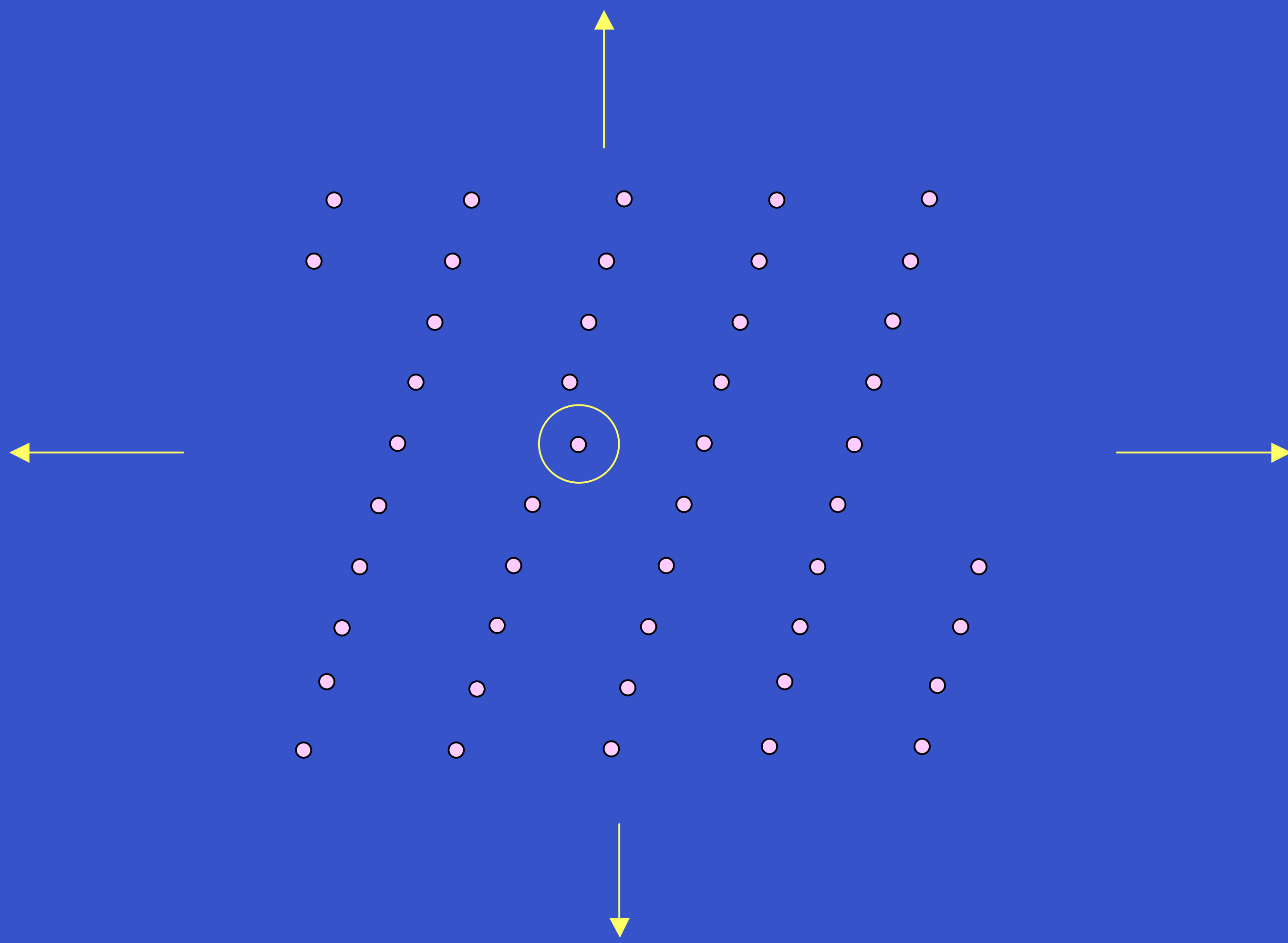
This array of points is a LATTICE (晶格)



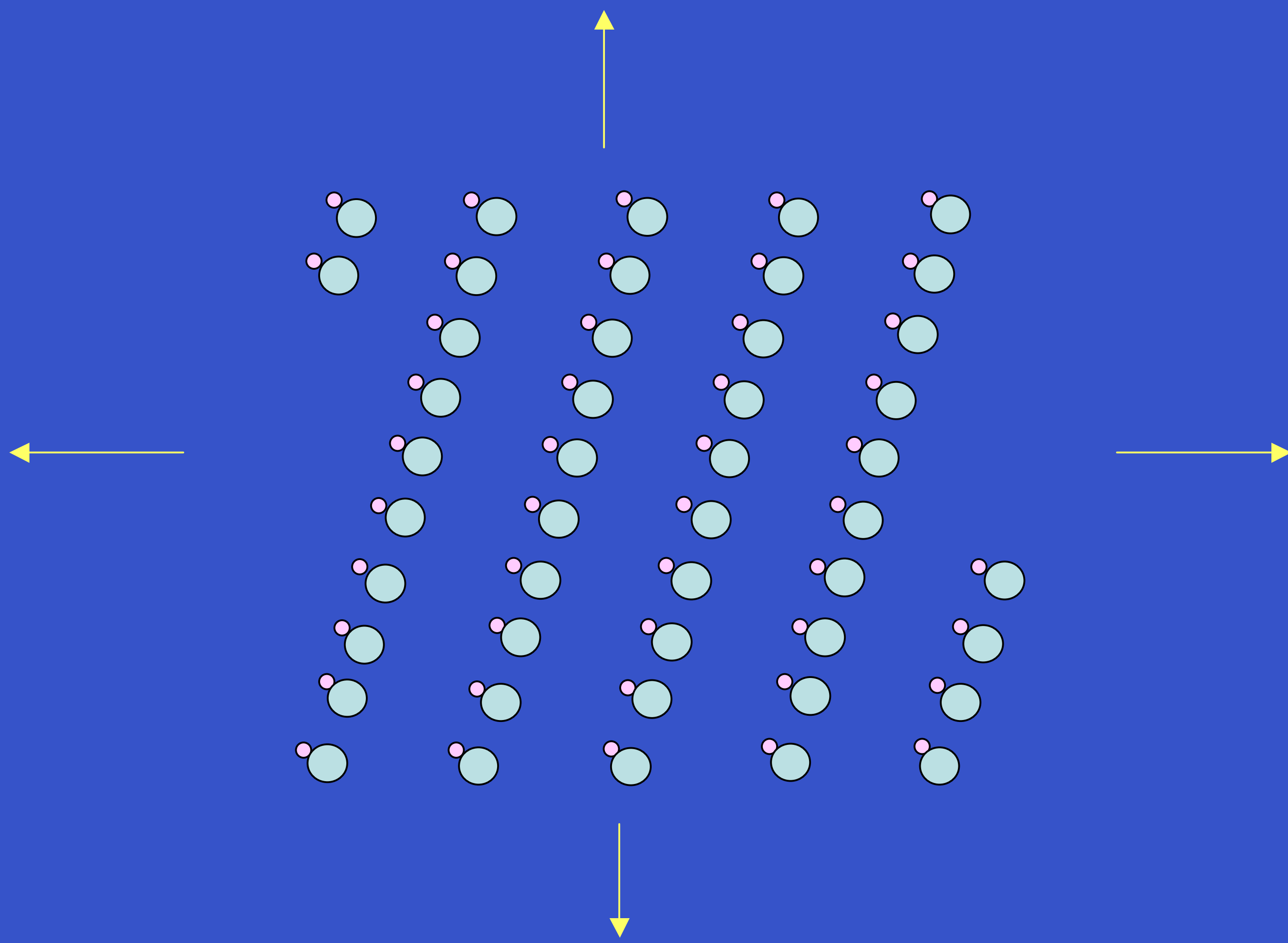
Lattice - infinite (无限的), perfectly periodic (周期性的) array of points in a space



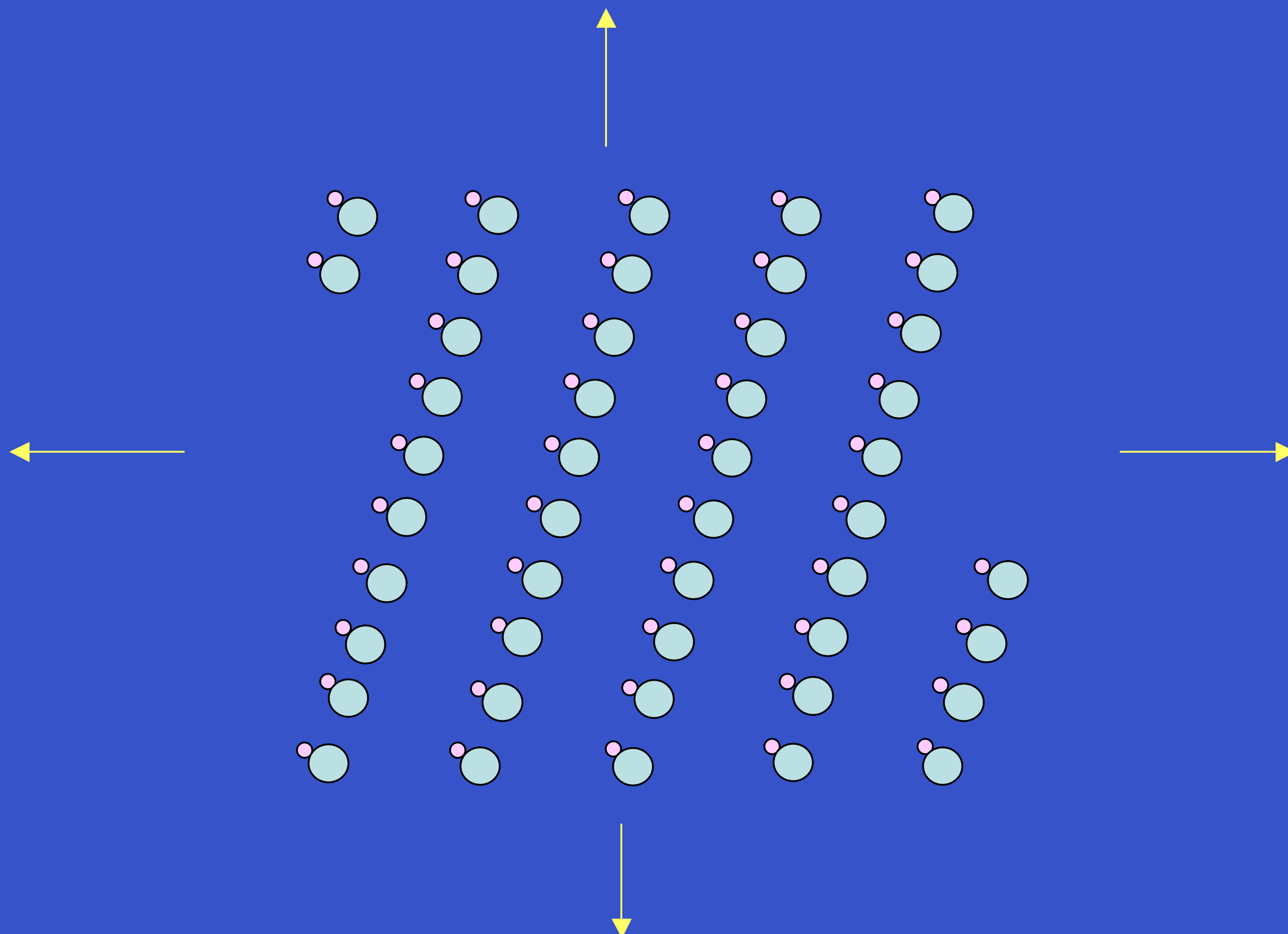
Not lattice:



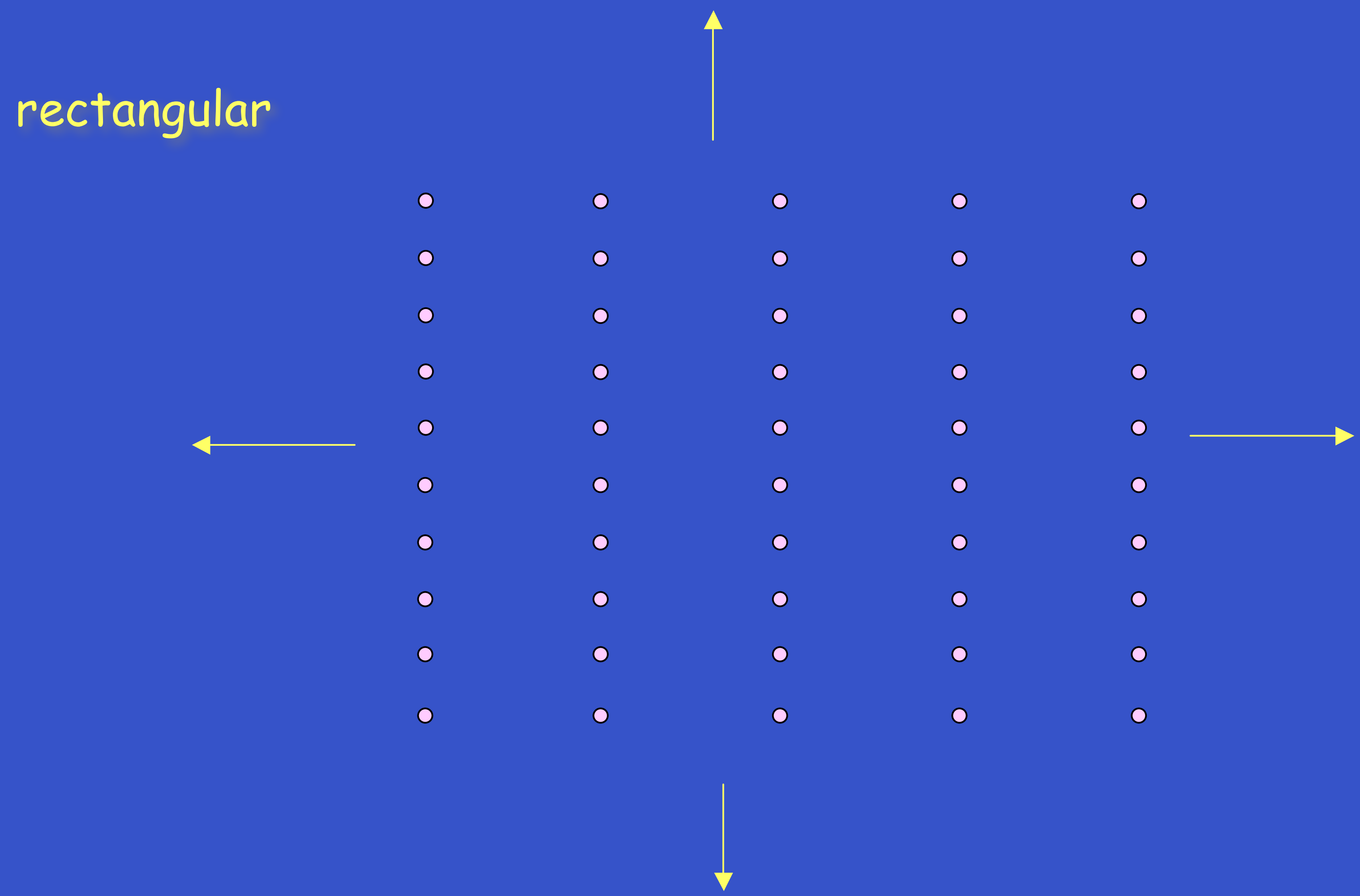
Not lattice:



Not lattice - ....some kind of STRUCTURE because not just points

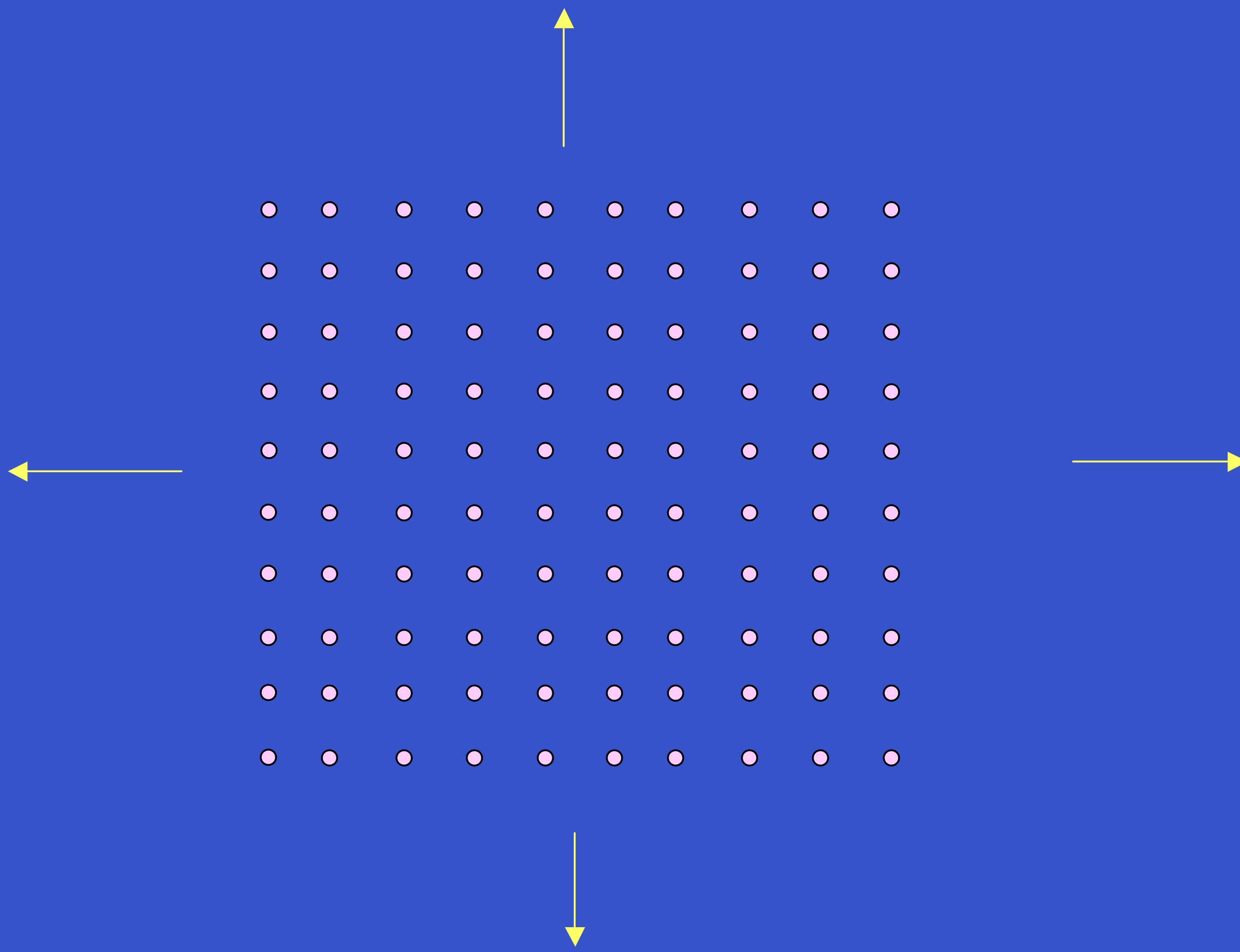


Another type of lattice - with different symmetry



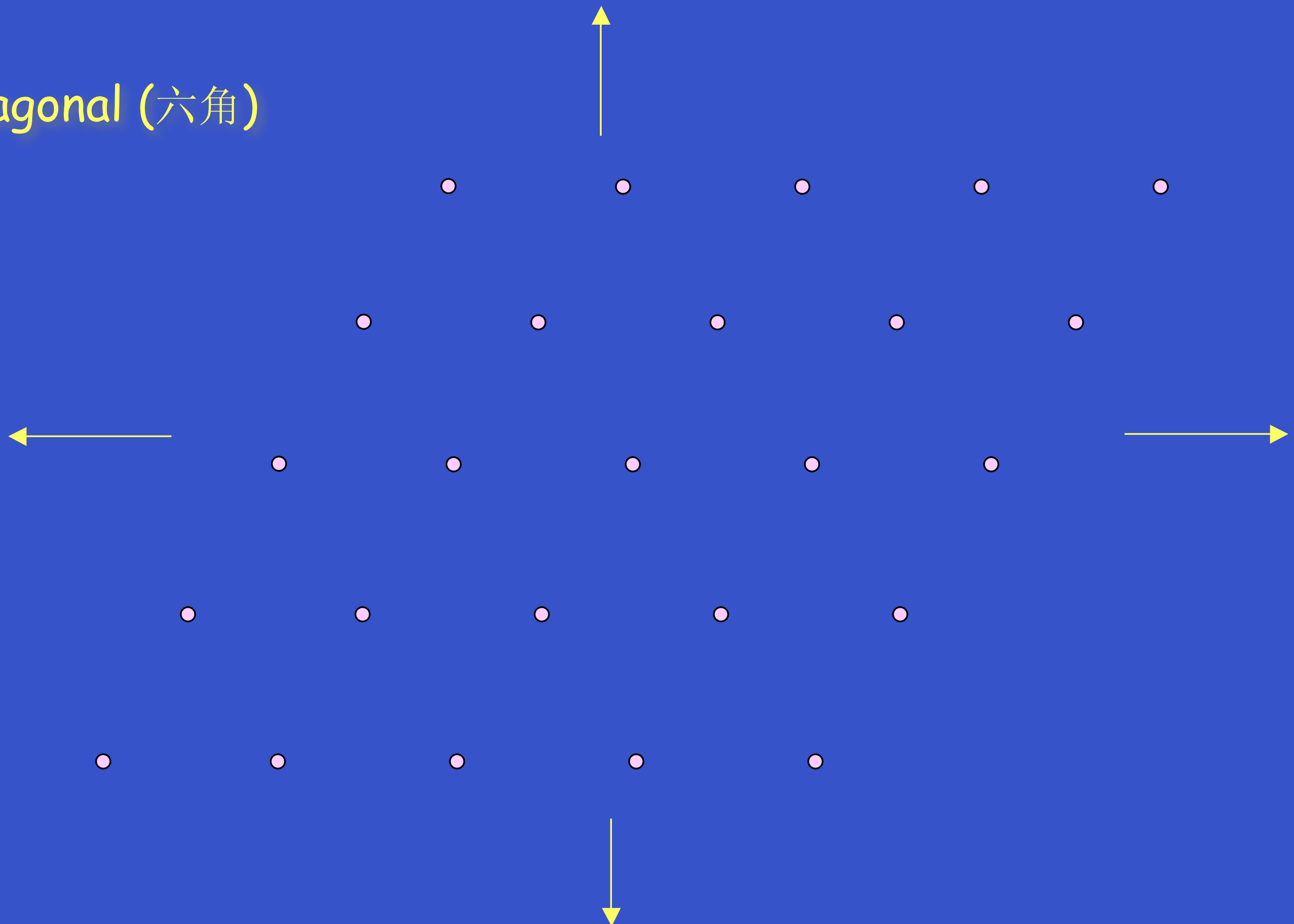
Another type of lattice - with different symmetry

square



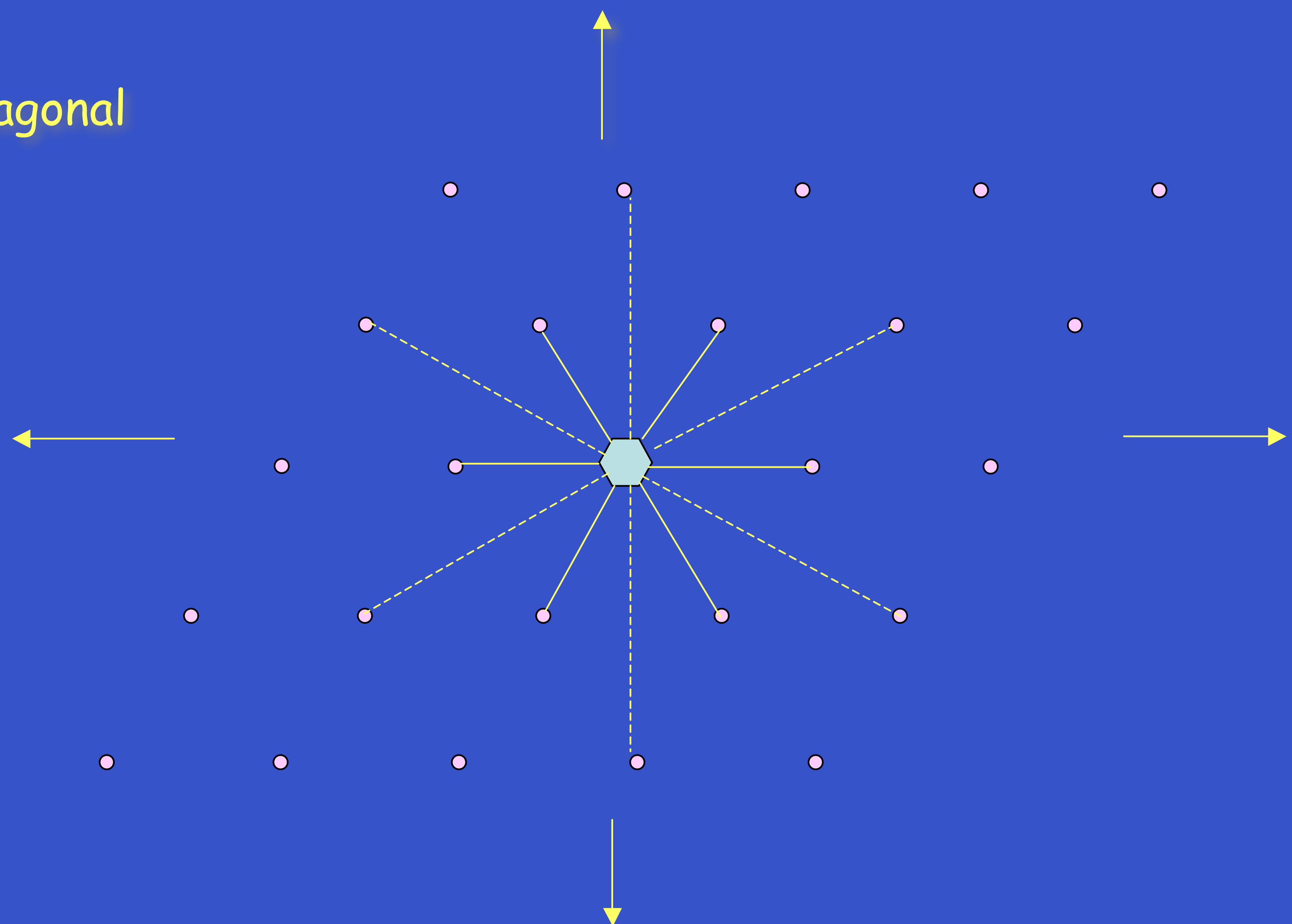
Another type of lattice - with different symmetry

hexagonal (六角)



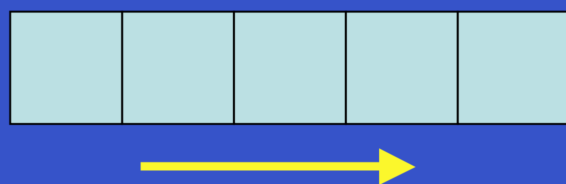
Back to rotation -
This lattice exhibits 6-fold symmetry

hexagonal

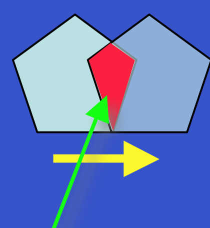


Periodicity and rotational symmetry

What types of rotational symmetry allowed?



object with 4-fold symmetry translates OK

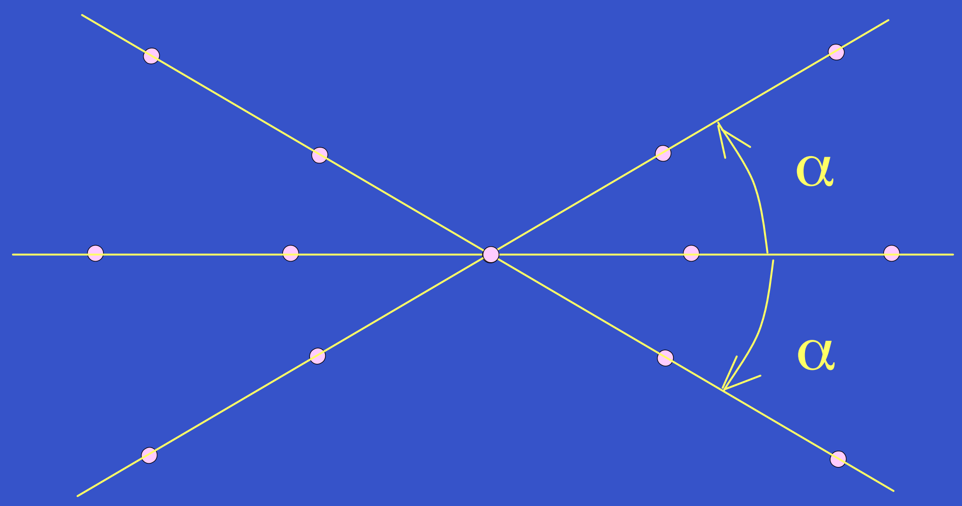


overlap not allowed

object with 5-fold symmetry doesn't translate

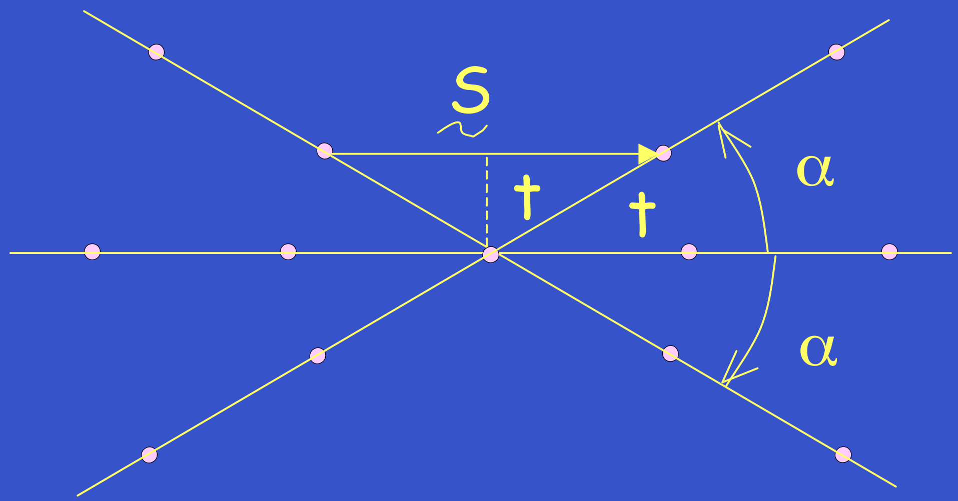
Periodicity and rotational symmetry

Suppose periodic row of points is rotated through $\pm\ \alpha$:

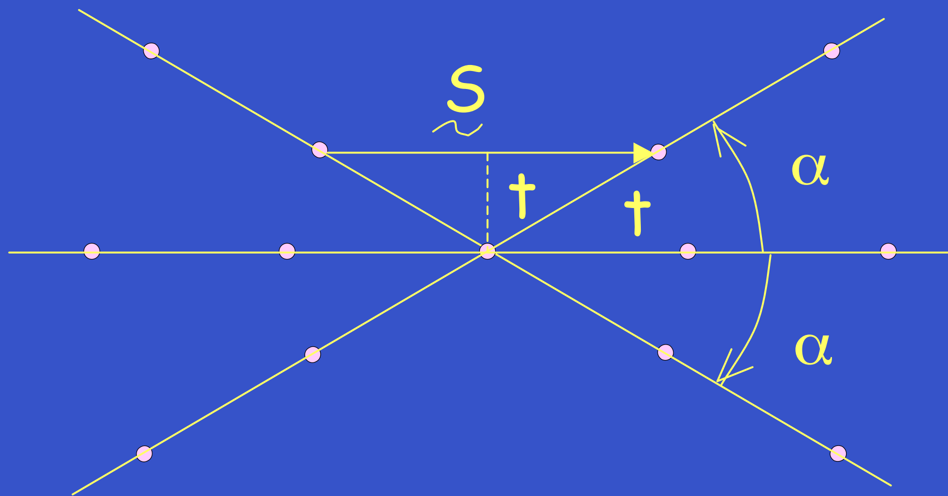


Periodicity and rotational symmetry

To maintain periodicity:



vector S = an integer x basis translation t



vector $\underset{\sim}{S}$ = an integer x basis translation $\underset{\sim}{t}$

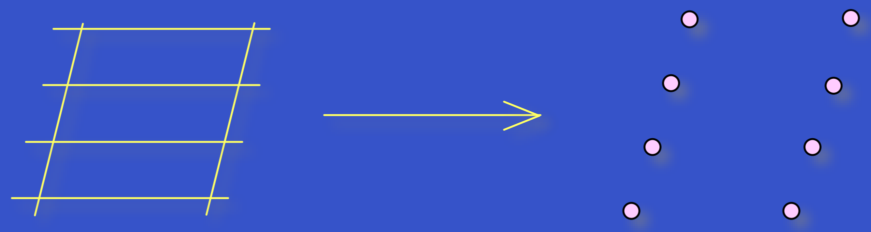
$t \cos\alpha = S/2 = mt/2$

m	cos α	α		axis
2	1	0	2 π	1
1	1/2	π/3	5π/3	6
0	0	π/2	3π/2	4
-1	-1/2	2π/3	4π/3	3
-2	-1	- π	π	2

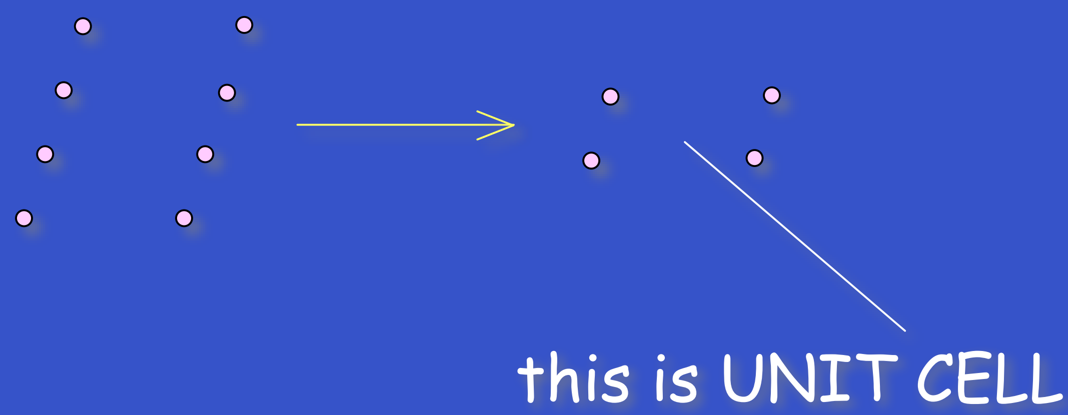
m	cos α	α		axis
2	1	0	2 π	1
1	1/2	π/3	5π/3	6
0	0	π/2	3π/2	4
-1	-1/2	2π/3	4π/3	3
-2	-1	- π	π	2

Only rotation axes consistent with lattice periodicity in 2-D or 3-D

We abstracted points from the shape:



Now we abstract further:



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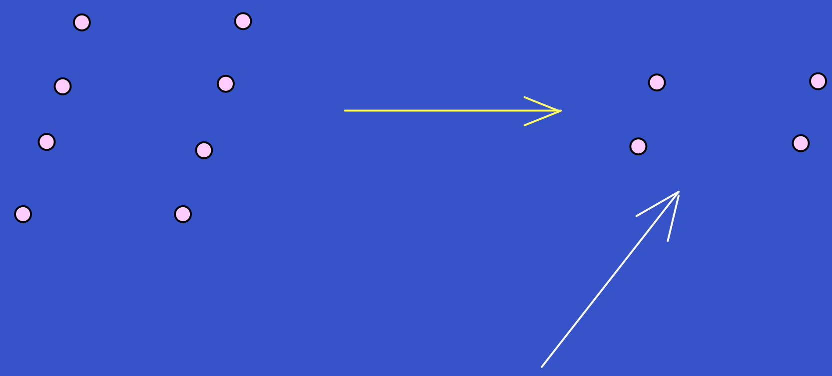
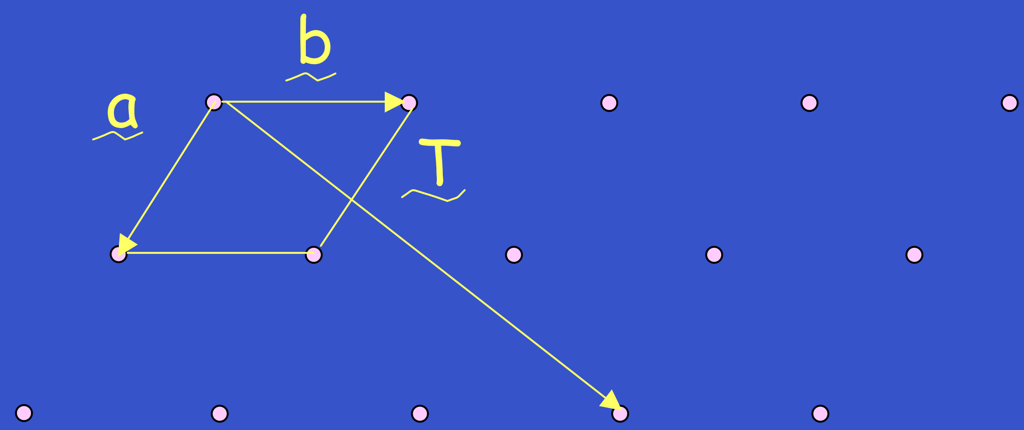


This is a UNIT CELL

Represented by two lengths and an angle

…….or, alternatively, by two vectors

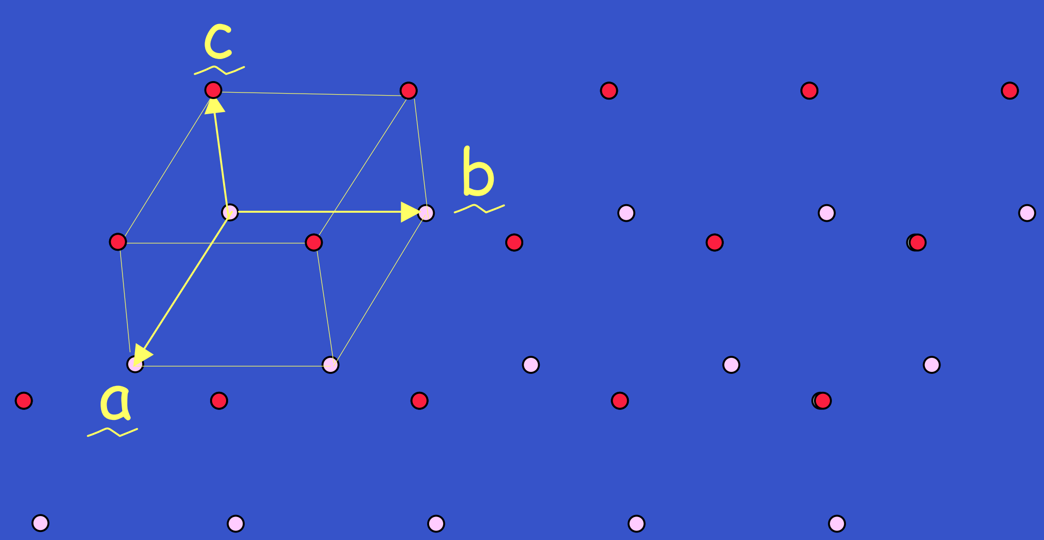
Basis vectors and unit cells



$$\underset{\sim}{T} = t_a\,\underset{\sim}{a} + t_b\,\underset{\sim}{b}$$

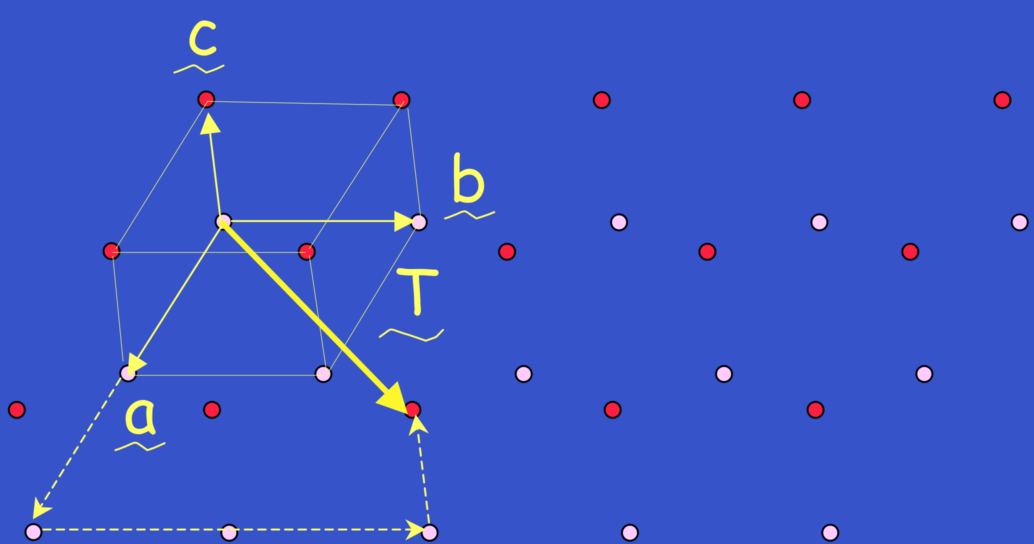
$\underset{\sim}{a}$ and $\underset{\sim}{b}$ are the basis vectors for the lattice

In 3-D:



a, b, and c are the basis vectors for the lattice

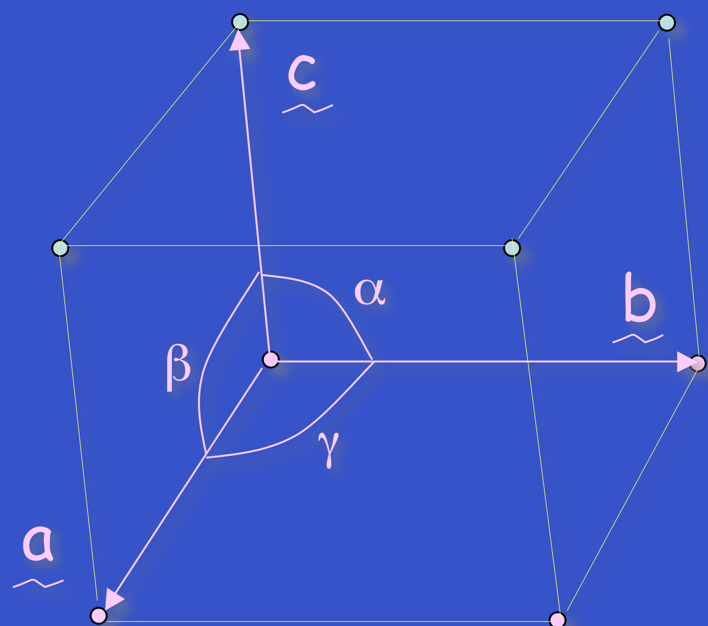
In 3-D:



$T = t_a\, a + t_b\, b + t_c\, c$ ---> [221] direction

a, b, and c are the basis vectors for the lattice

Lattice parameters (晶格参数) :



need 3 lengths - |a|, |b|, |c|

& 3 angles - α, β, γ

to get cell shape & size

The many thousands of lattices classified into **crystal systems** (晶系)

System	Interaxial Angles	Axes
Triclinic	$\alpha \neq \beta \neq \gamma \neq 90°$	$a \neq b \neq c$
Monoclinic	$\alpha = \gamma = 90° \neq \beta$	$a \neq b \neq c$
Orthorhombic	$\alpha = \beta = \gamma = 90°$	$a \neq b \neq c$
Tetragonal	$\alpha = \beta = \gamma = 90°$	$a = b \neq c$
Cubic	$\alpha = \beta = \gamma = 90°$	$a = b = c$
Hexagonal	$\alpha = \beta = 90°, \gamma = 120°$	$a = b \neq c$
Trigonal	$\alpha = \beta = 90°, \gamma = 120°$	$a = b \neq c$

The many thousands of lattices classified into

crystal systems

System	Minimum symmetry
Triclinic	1 or $\bar{1}$
Monoclinic	2 or $\bar{2}$
Orthorhombic	three 2s or $\bar{2}$s
Tetragonal	4 or $\bar{4}$
Cubic	four 3s or $\bar{3}$s
Hexagonal	6 or $\bar{6}$
Trigonal	3 or $\bar{3}$

For given lattice, infinite number of unit cells possible: