Lecture 2

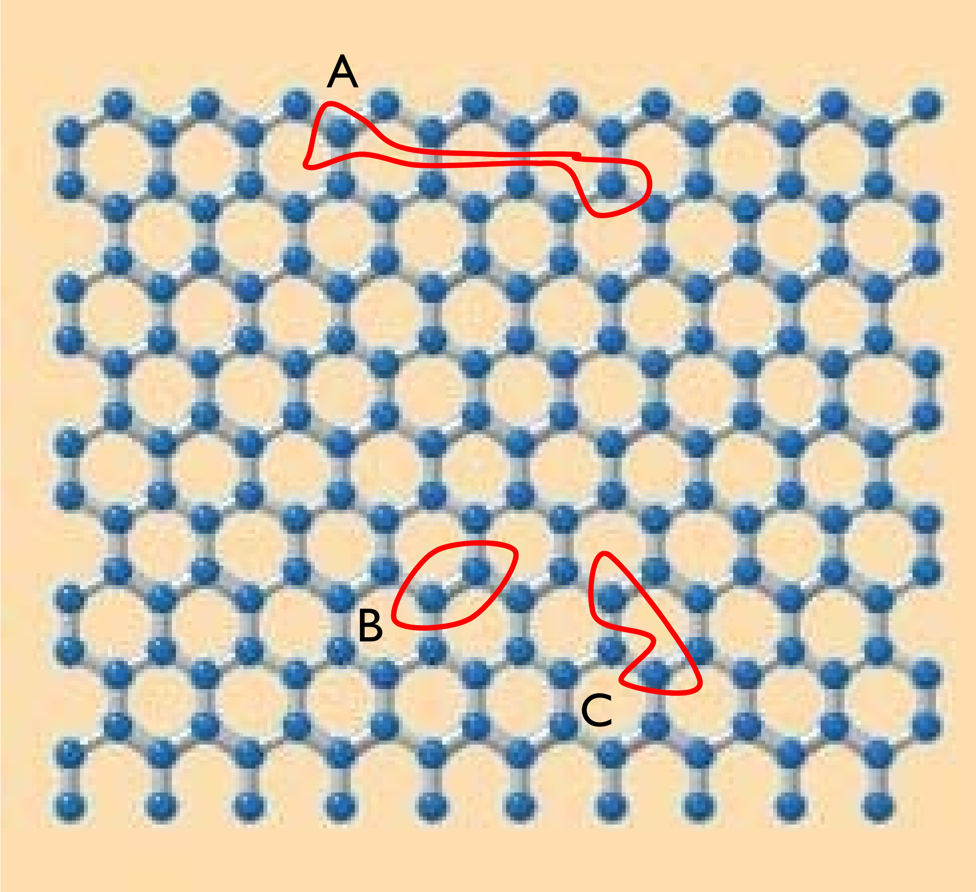
Basic crystallography (continued)

Crystals happen

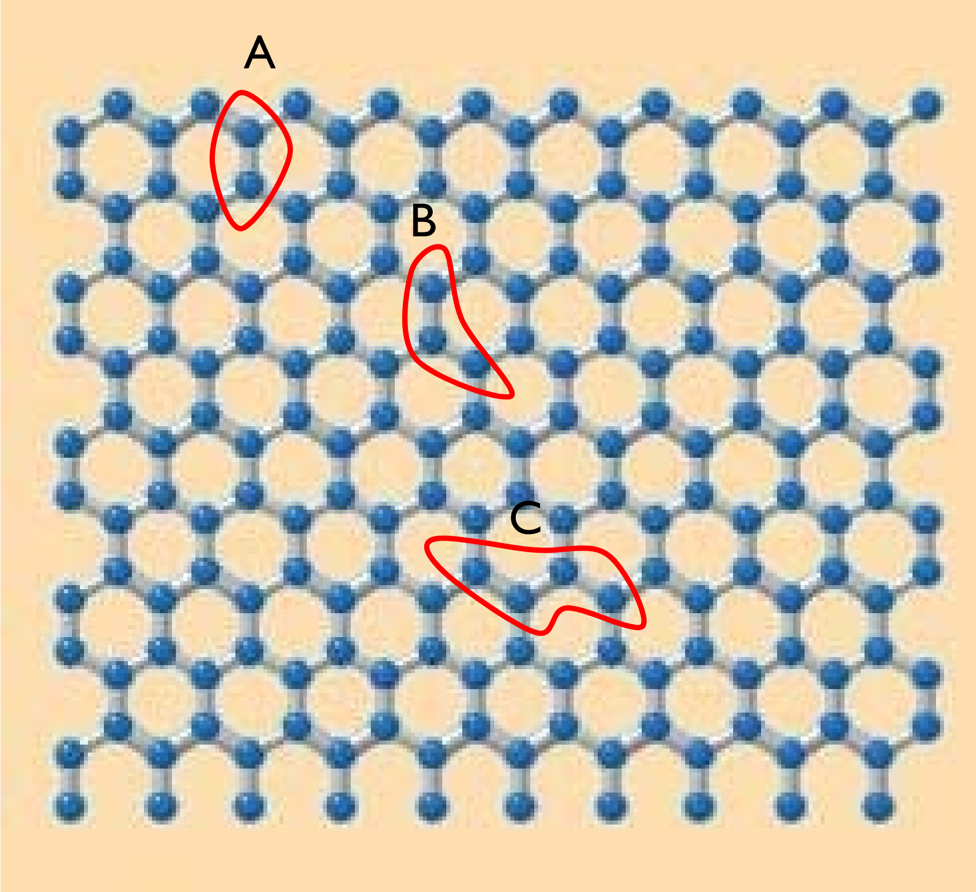
basic emergent phenomenon
"ordering" of many body system

How it happens is hard to know, but one can study what happens – this is the subject of crystallography

Q1. Which of these is not a basis for graphene?

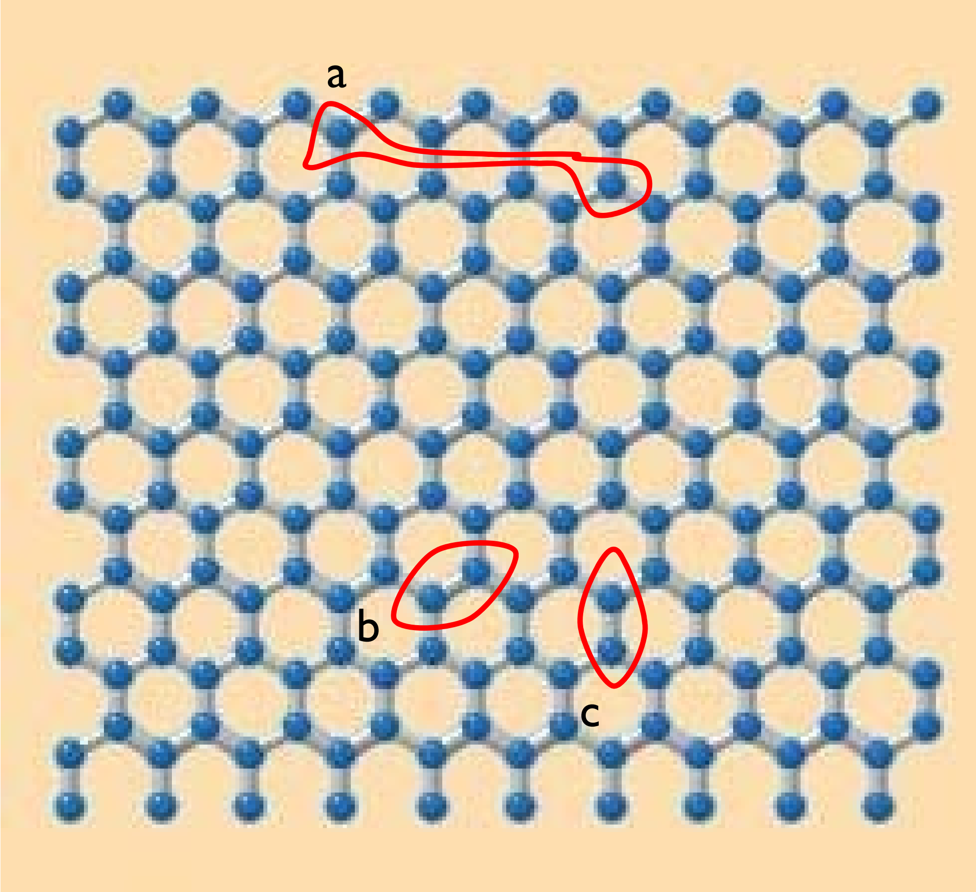


Q2. Which of these is not a basis for graphene?



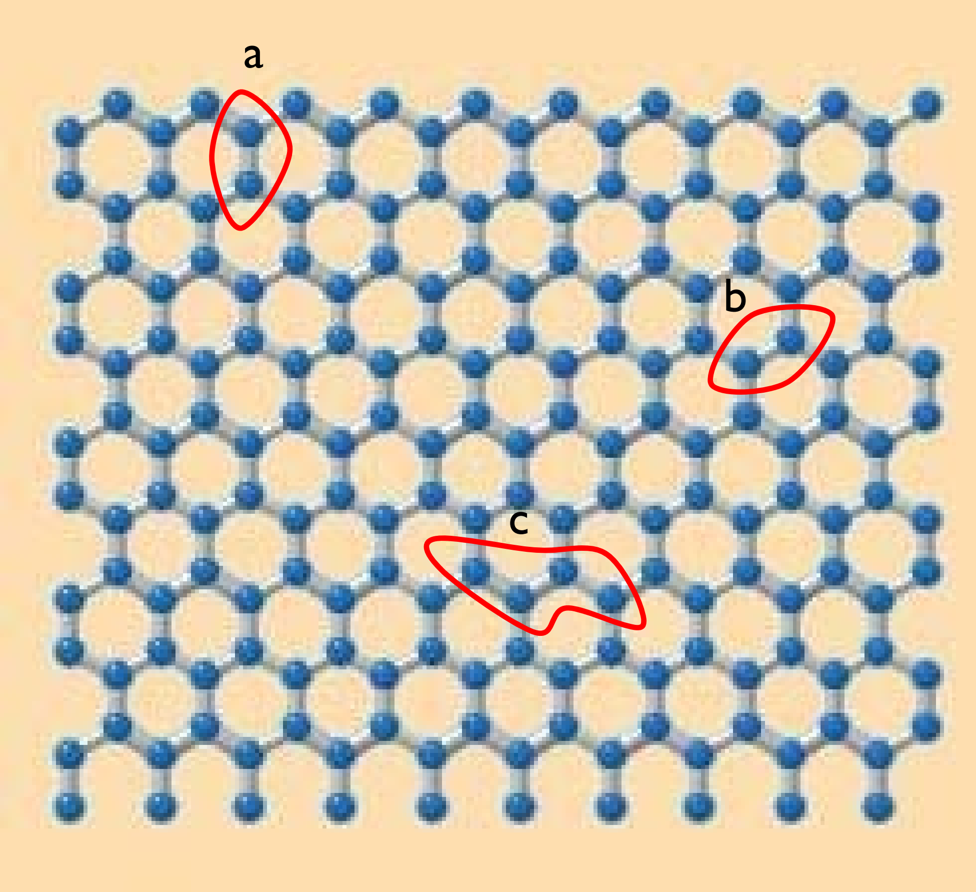
Q3. Is it possible to define the same Bravais lattice for these different basis choices a,b,c?

A. Yes B. No C. Depends



Q4. Is it possible to define the same Bravais lattice for these different basis choices a,b,c?

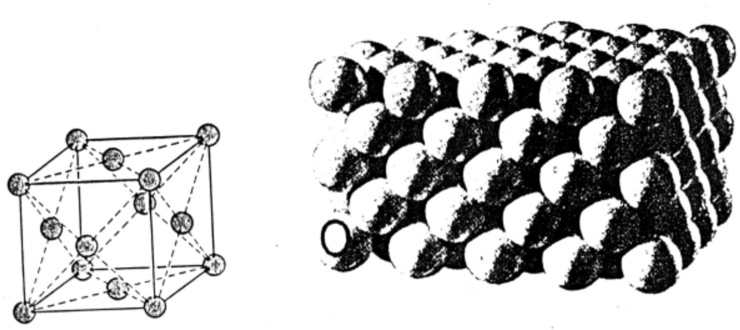
A. Yes B. No C. Depends



Q5. FCC and HCP (hexagonal-close-packed) crystals are shown below. The number of balls (“atoms”) in the primitive basis is respectively:

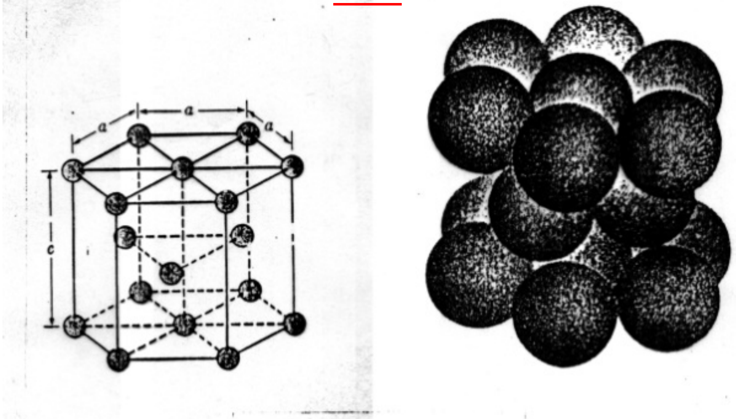
A. 1,1 B. 1,2 C. 2,2

FCC (CCP)



Face Centered Cubic Lattice

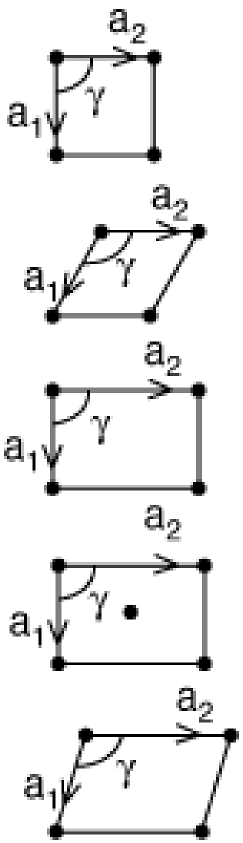
HCP



Hexagonal Lattices

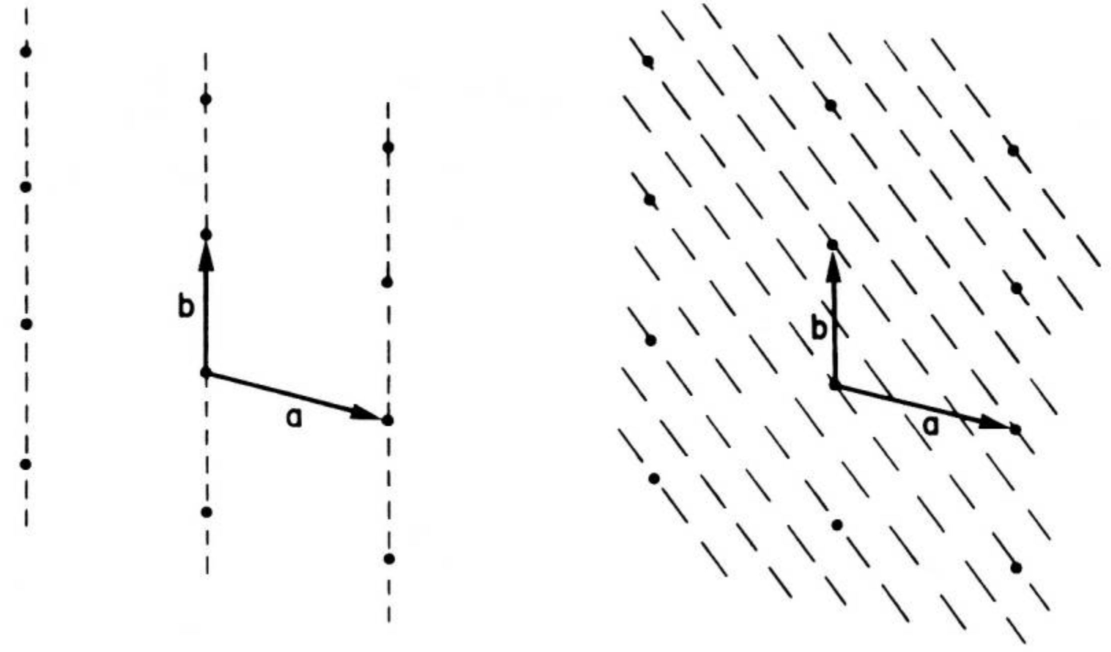
http://www.ae.iitm.ac.in/~sriram/as401/materials

DQ1. These are all possible two-dimensional Bravais Lattices. For hexagonal and oblique, show what the Wigner-Seitz cell (pages 13,14) looks like.



square	$a_1 = a_2$	$\gamma = 90°$
hexagonal	$a_1 = a_2$	$\gamma = 120°$
rectangular	$a_1 \neq a_2$	$\gamma = 90°$
centered rectangular	$a_1 \neq a_2$	$\gamma = 90°$
oblique	$a_1 \neq a_2$	$\gamma \neq 60°, 90°, 120°$

DQ2. Using this picture (Figure 1.5), explain the concept of a "lattice plane" and "Miller indices". (first part of section 1.2.3) What is the relation between the density of atoms in the lattice plane and the spacing between lattice planes? The (rough) relation between the "magnitude" of Miller indices and the spacing? Explain why lattice planes are Bravais lattices (in a lower dimension) by themselves.



Crystal Resources on the Web

- Crystal Group

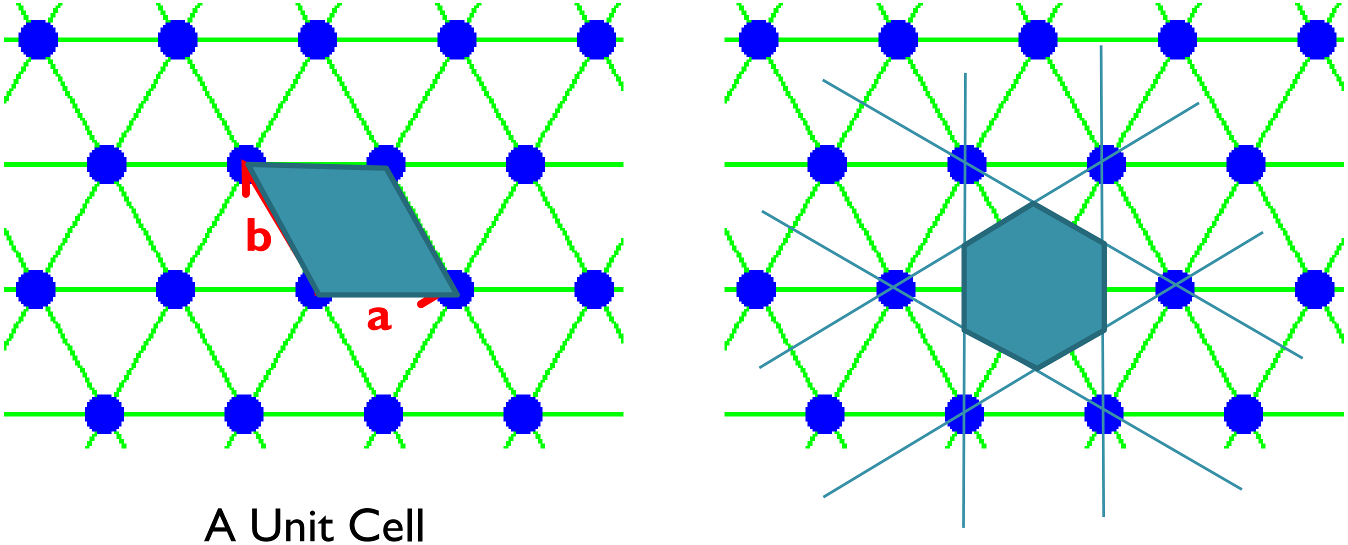
  e.g. http://img.chem.ucl.ac.uk/sgp/mainmenu.htm
- Real crystal struct. data base (real compounds)

  e.g. http://icsd.ill.fr/icsd/index.html

Unit cell

- Repeating (and exactly space-filling) geometry assigned to each <u>lattice</u> point

Bravais Lattice (NOT crystal) of graphene



A Unit Cell

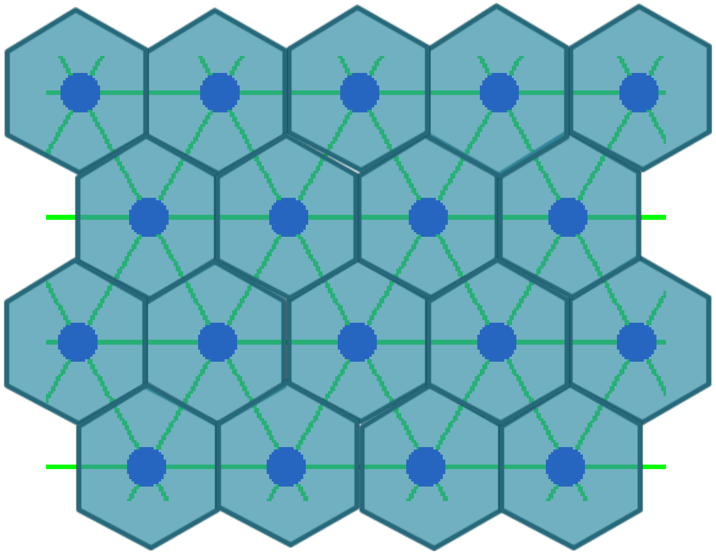
http://home.hetnet.nl/~turing/complete_hex_motif_2a.gif

<u>Wigner Seitz Unit Cell</u>
(Hexagon in this case)

Wigner Seitz cell is the "the most natural" or "the nicest"

- Reflects all symmetries of the lattice itself

(why? – too advanced math for this class, but physically one can think of the WS cell as the "imprint" of the environment)



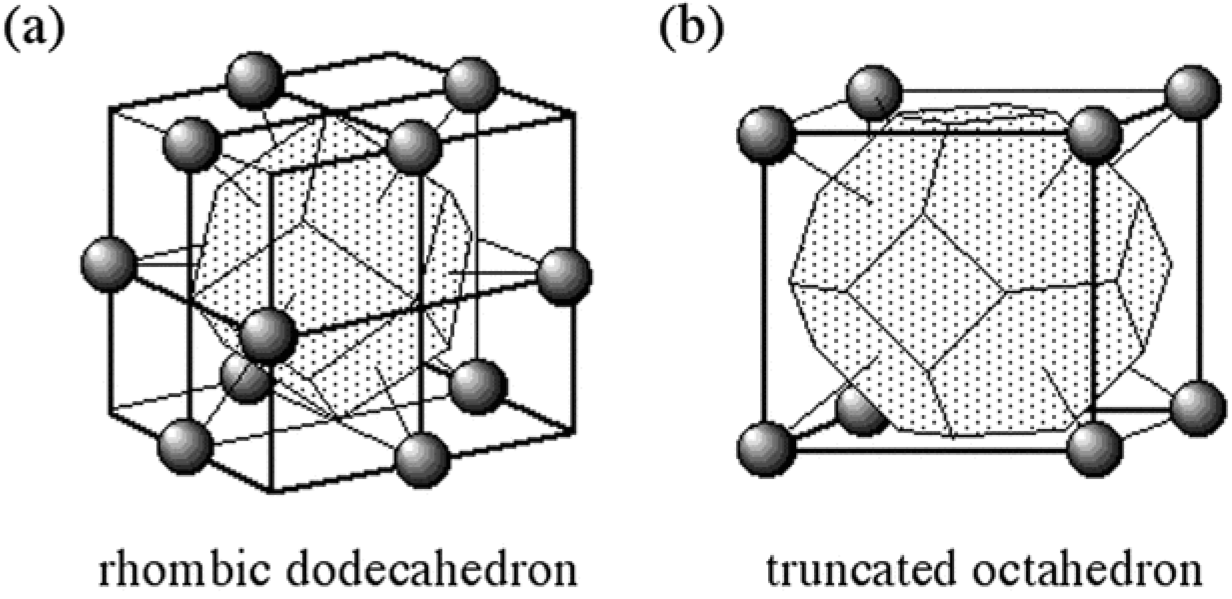
Wigner Seitz Unit Cell

Imagine each blue ball is a balloon (or play dough) which is inflated at the same time. Eventual shape of each ball will be the WS cell – an "imprint" of its neighbors for each lattice point . This is why.

Examples of Wigner Seitz Cells for 3d Lattices

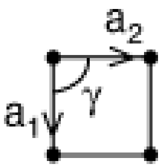
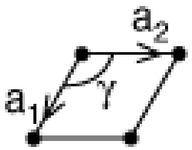
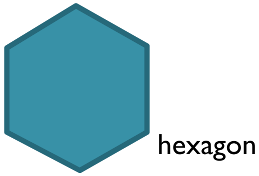
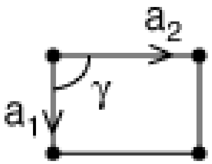
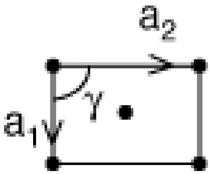
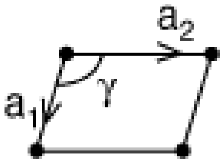
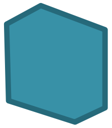
Face centered cubic (fcc)
(note that the origin is shifted)

Body centered cubic (bcc)



http://journals.iucr.org/j/issues/2003/04/00/ks7313/ks7313fig6.html

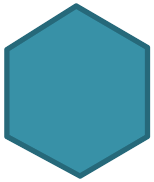
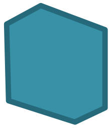
Classification of Lattice (2d)

				WS Cell Shape	Symmetry
	square	$a_1 = a_2$	$\gamma = 90^\circ$		4, v, h, i
	hexagonal	$a_1 = a_2$	$\gamma = 120^\circ$		6, v, h, i
	rectangular	$a_1 \neq a_2$	$\gamma = 90^\circ$		2, v, h, i
	centered rectangular	$a_1 \neq a_2$	$\gamma = 90^\circ$		2, v, h, i
	oblique	$a_1 \neq a_2$	$\gamma \neq 60^\circ, 90^\circ, 120^\circ$		2, i

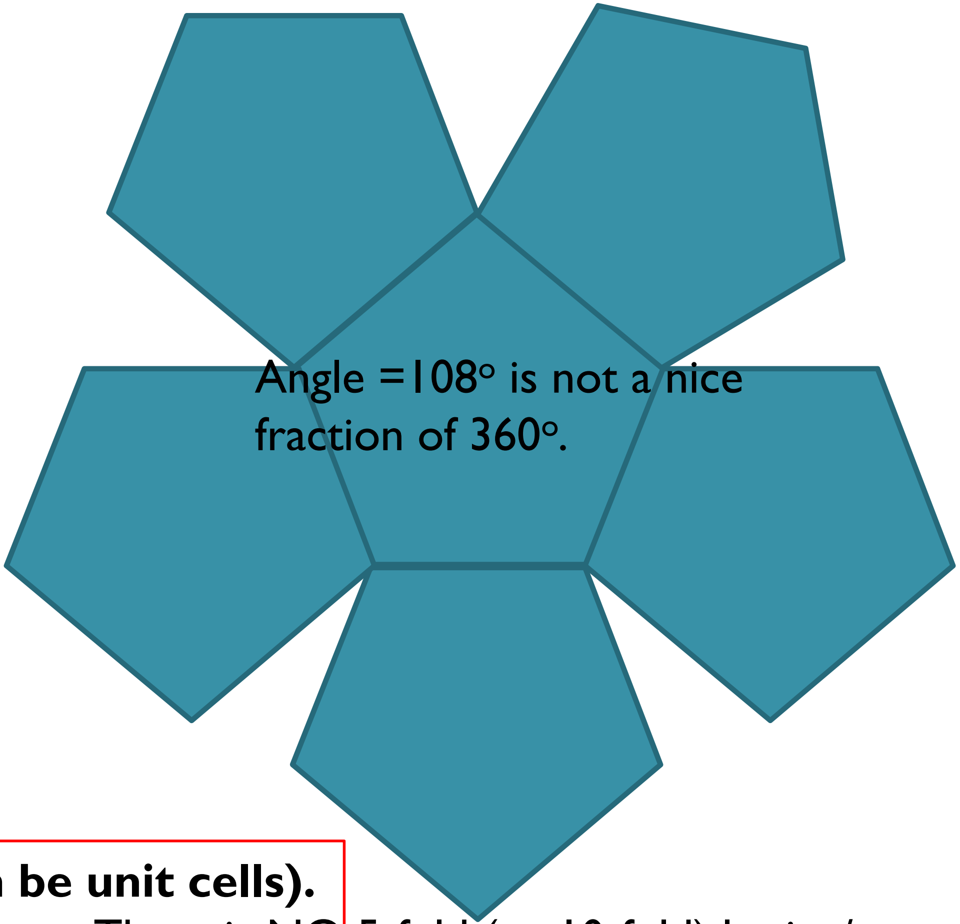
http://whome.phys.au.dk/~philip/q1_05/surflec/fig6_5.gif

2,4,6 = 2,4,6-fold rotation
v = vertical reflection
h = horizontal reflection
i = inversion

These are all WS cell shapes in 2d

WS Cell Shape	Symmetry
 square	4, v, h, i
 hexagon	6, v, h, i
	2, v, h, i
	2, v, h, i
	2, i

Why not (regular) pentagon?



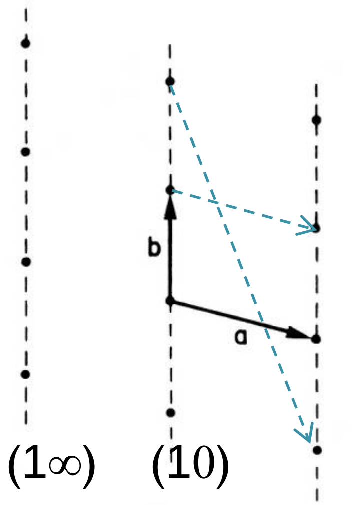
Angle =108° is not a nice fraction of 360°.

These can fill space (i.e. can be unit cells).
But a pentagon cannot.

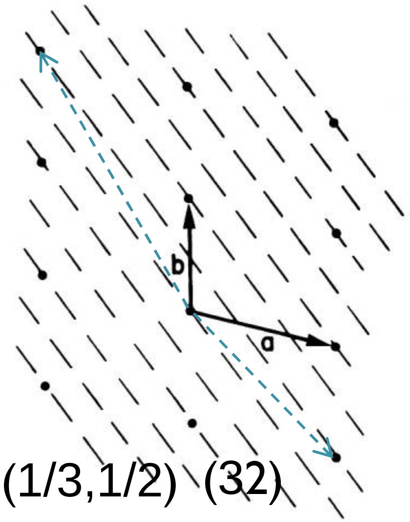
There is NO 5-fold (or 10-fold) lattice/crystal.

Lattice Planes and Miller Indices

- A d-dimensional lattice can be decomposed into identical (d-1)-dimensional lattices (“lattice planes”)



(10) or $(\bar{1}0)$ plane
+ one of --> = lattice



(32) or $(\bar{3}\bar{2})$ plane
+ one of --> = lattice

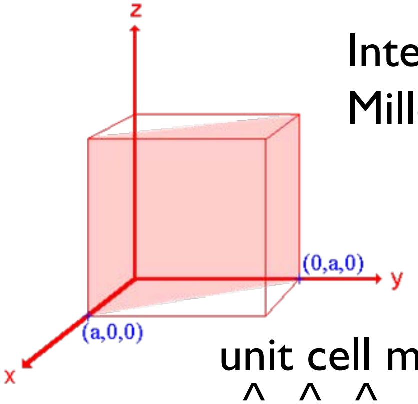
- **Miller Indices**
1. **Draw unit vectors of the lattice (origin defined).**
2. **Identify the plane that come closest to, but does not cross, origin.**
3. **Write down the intercepts with the unit vectors (non-Cartesian in general!)**
4. **Make an inverse.**
5. **Minus sign goes as bar on top.**

- Lattice plane is described by <u>Miller indices</u>

Notation for planes (Miller indices) and directions

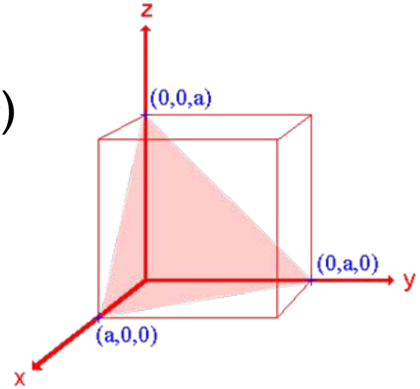
Intercepts with unit vector axes (not cartesian, in general !)

Cubic Lattice Example
(principle the same for all lattices)

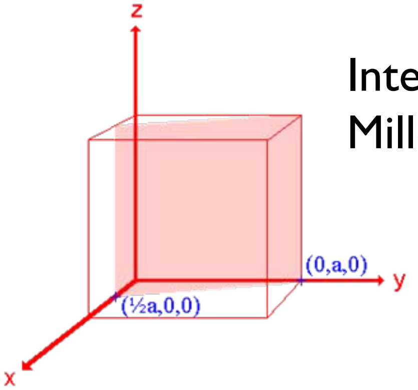


Intercepts: 1,1,∞
Miller indices: (110)

unit cell made from
$a\hat{x}$, $a\hat{y}$, $a\hat{z}$



Intercepts: 1,1,1
Miller indices: (111)



Intercepts: ½, 1, ∞
Miller indices: (210)

{uvw} = group index (all equivalents)
Example:
$\{1\ 0\ 0\} = (100)(010)(001)(\bar{1}00)(0\bar{1}0)(00\bar{1})$

bar means minus

Direction notation = [uvw]
means u**a** + v**b** + w**c**
(u, v, w are integers)

http://www.chem.qmul.ac.uk/surfaces/scc/scat1_1b.htm