Lecture 1

Basic crystallography

Crystals happen

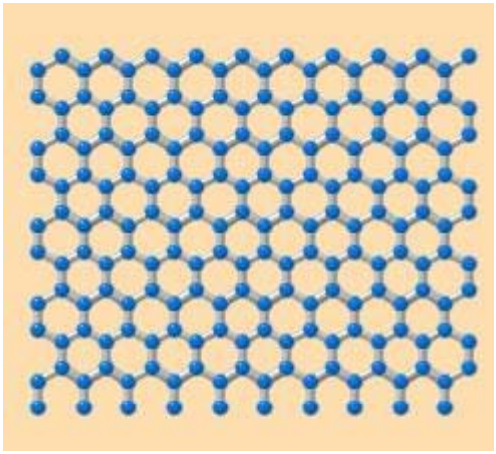
basic emergent phenomenon
"ordering" of many body system

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

Learning question 1

Page 3 of H&H

- Crystal means something that repeats
  Something = Basis
  Repetition = Lattice
  (Bravais Lattice, Crystal Lattice)
- How to define basis and lattice is not unique for a given crystal.
- For the graphene lattice, explain **basis, lattice**, and explain whether the lattice is **primitive**.

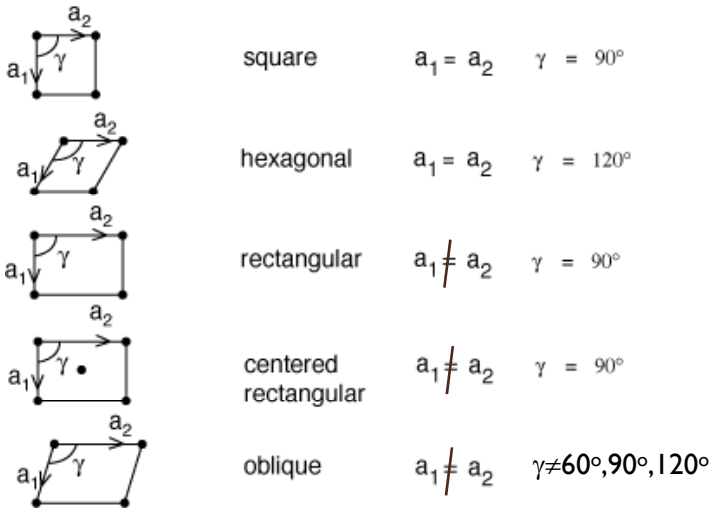


http://www.ahwahneetech.com

Learning question 2

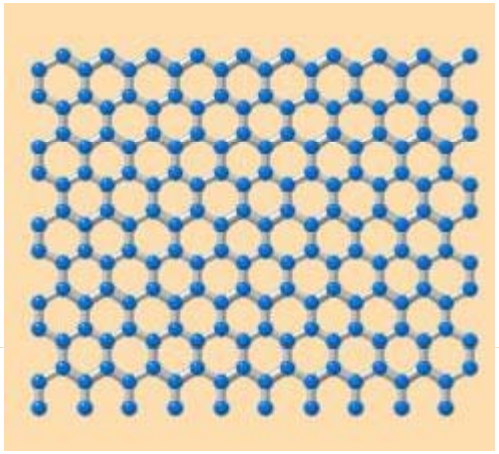
Pages 6,7 of H&H

- Explain Figure 1.4 of Hook and Hall.
- Explain what are point symmetries of each lattice. (rotation, reflection, inversion)
- Obtain the **Wigner Seitz unit cell** (see Figure 1.10 and page 13) for each of these, and show that the WS cell has all symmetries noted above.



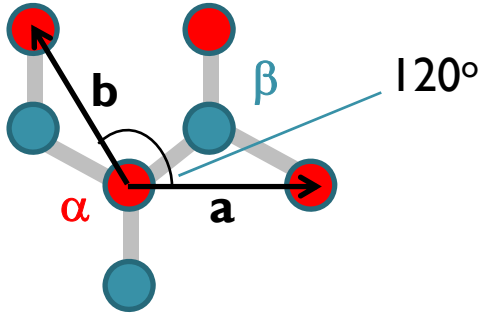
http://whome.phys.au.dk/~philip/q1_05/surflec/fig6_5.gif

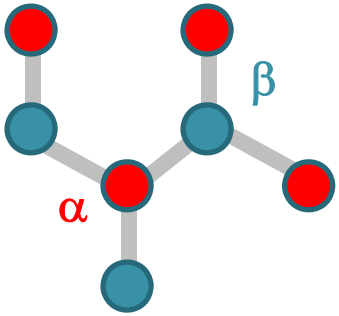
Crystal = basis and lattice



"Honeycomb" of graphene
Repeated "Benzene" ring
Each C atom is shared by three rings
Two C atoms per benzene ring
I.e. there are two C atoms per basis
Or, there are two inequivalent C atoms

http://www.ahwahneetech.com





Basis = α + β
Lattice = defined by unit vectors **a, b**
|**a**|=|**b**|, angle = 120°, **hexagonal (or triangular) lattice**
This lattice is a **primitive lattice**, i.e. its basis is not redundant.

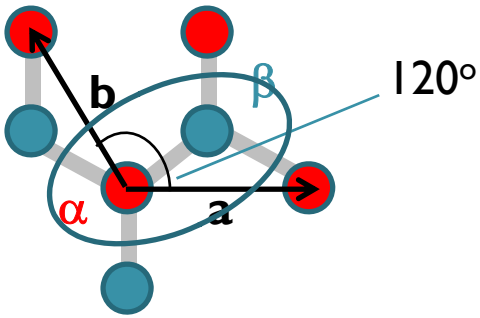
Mathematically speaking …

Lattice ≡ u **a** + v **b,** u, v = integers
(For 3d, lattice ≡ u **a** + v **b** + w **c**, where u, v, w = integers)

a, b = lattice vectors

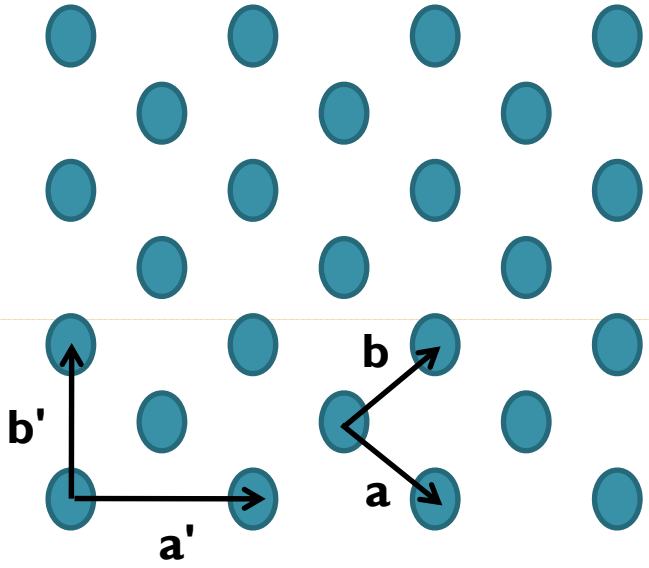
Basis is then specified by fractional numbers in general

Example:



Basis coordinates:
0 **a** + 0 **b**
(2**a** + **b**)/3

Crystal = basis + lattice



Centered rectangular lattice

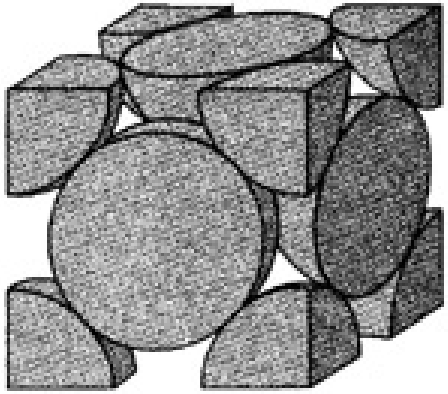
Primitive lattice is given by,
e.g., **a, b**
|**a**|=|**b**|, angle ≠ 60°, 90°, 120°
Single atom basis

Or, a lattice can be defined by
a', b' and two atom basis

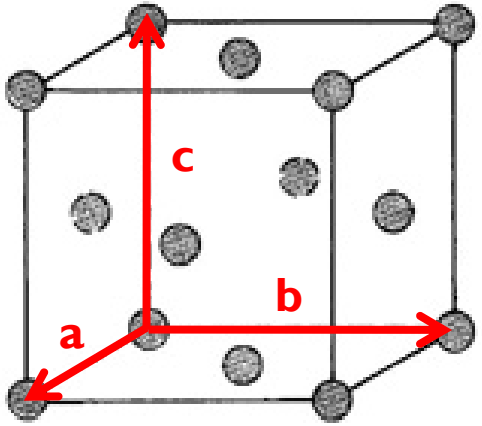
Which lattice to choose is out of convention and preference.
Often a non-primitive lattice used extensively is called a **conventional lattice**.

Conventional lattice and Primitive lattice

Face Centered Cubic Lattice (fcc)

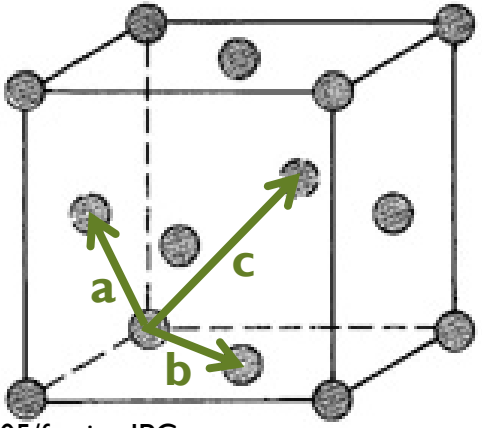


Four Atom Basis



Conventional (Cube)
|a| = |b| = |c|
All angles 90°

Four Atom Basis



Primitive (Rhombohedron)
|a| = |b| = |c|
All angles 60°

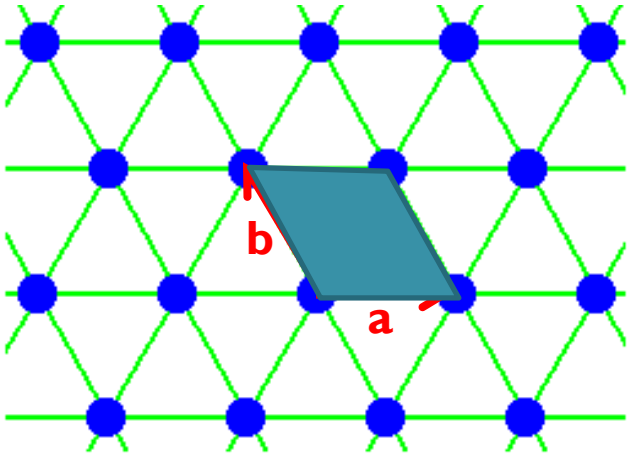
Single Atom Basis

http://info.lu.farmingdale.edu/depts/met/met205/fcc-jpg.JPG

Unit cell

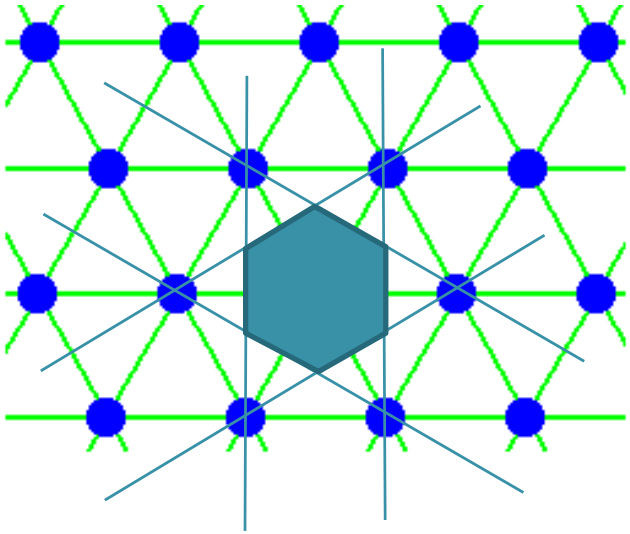
- Repeating geometry assigned to each lattice point

Lattice (NOT crystal) of graphene



A Unit Cell

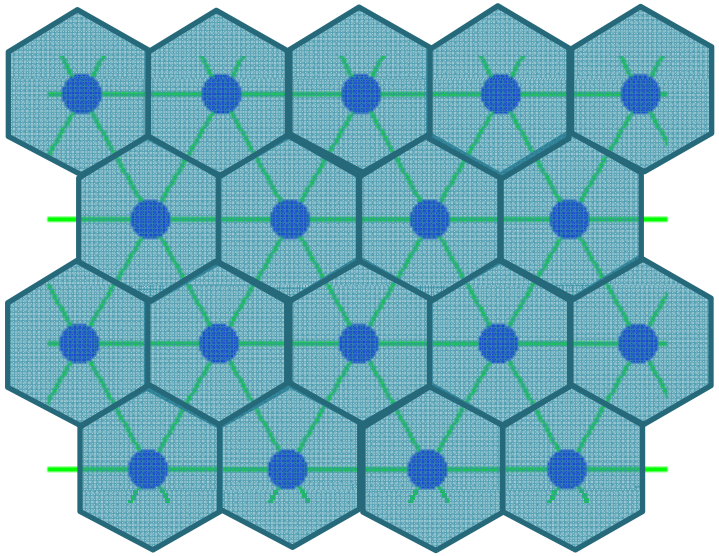
http://home.hetnet.nl/~turing/complete_hex_motif_2a.gif



Wigner Seitz Unit Cell
(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)



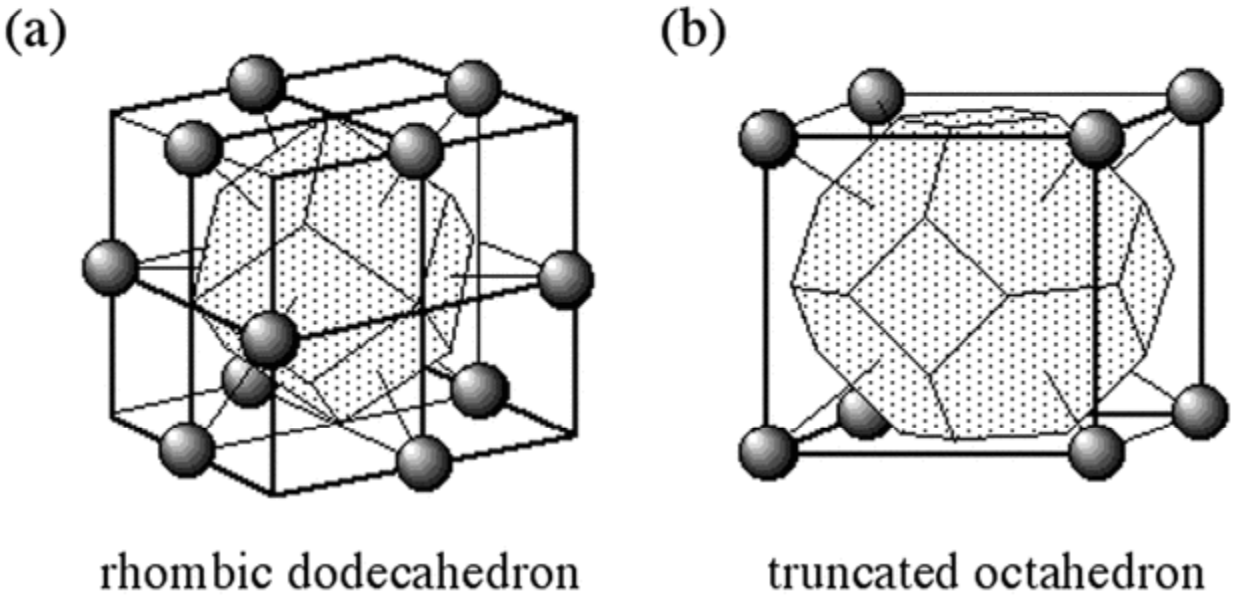
Wigner Seitz Unit Cell

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

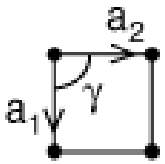
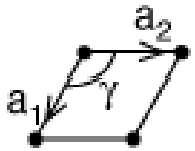
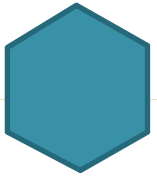
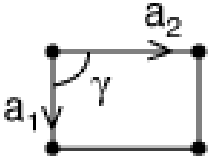
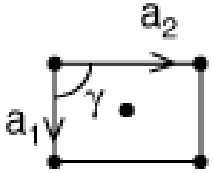
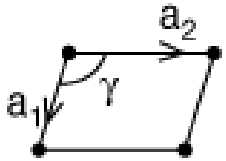
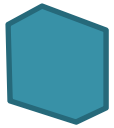
Face centered cubic (fcc)
(note that the origin is shifted)

Body centered cubic (bcc)



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

Classification of Lattice (2d)

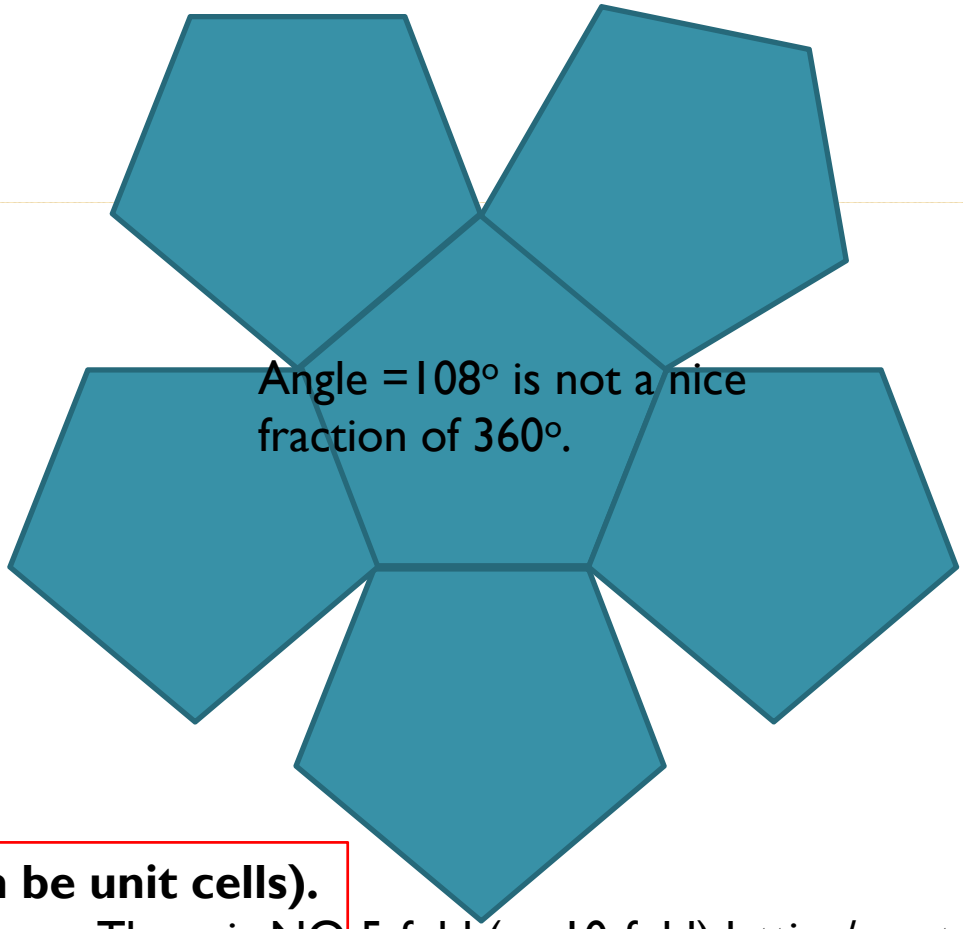
			WS Cell Shape	Symmetry
	square	$a_1 = a_2$ $\gamma = 90°$	 square	4, v, h, i
	hexagonal	$a_1 = a_2$ $\gamma = 120°$	 hexagon	6, v, h, i
	rectangular	$a_1 \neq a_2$ $\gamma = 90°$		2, v, h, i
	centered rectangular	$a_1 \neq a_2$ $\gamma = 90°$		2, v, h, i
	oblique	$a_1 \neq a_2$ $\gamma \neq 60°, 90°,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

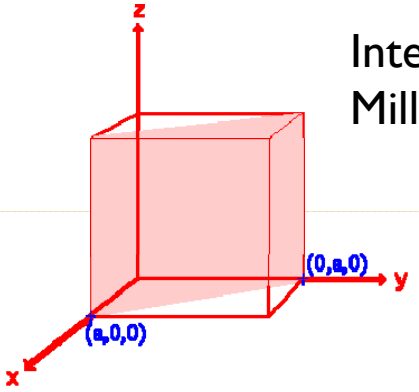


These can fill space (i.e. can be unit cells).
But a pentagon cannot.

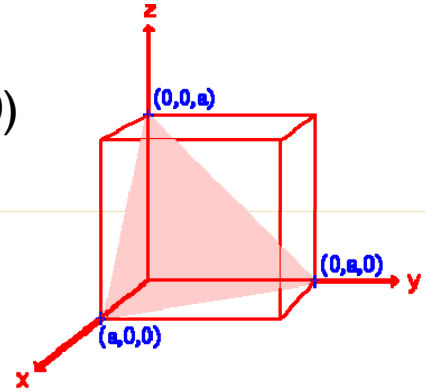
There is NO 5-fold (or 10-fold) lattice/crystal.

Notation for planes (Miller indices) and directions

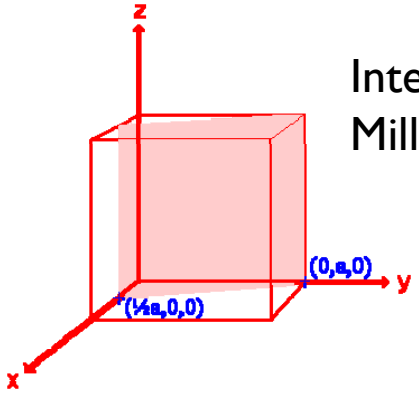
Cubic Lattice Example
(principle the same for all lattices)



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



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