Lecture 3
Crystal Lattices

Structural/Atomic [Form] Factors and Point/Space Groups

- Everything here continues to be static

  i.e. [quantum] jitters of atoms are complete

  ignored

Structural Factor and Atomic Form Factor

X-Ray Scattering Amplitude is given by

$\sum_{\mathbf{R}} \exp(i\, \mathbf{q} \cdot \mathbf{R}) \sum_{\mathbf{j}} f_j(\mathbf{q}) \exp(i\, \mathbf{q} \cdot \mathbf{r}_j)$

(j = index running over atoms in the basis)

The 2nd summation is called a structural factor (S_K) and $f_j(K)$ is an atomic form factor

$$S_K = \sum_{\mathbf{j}} f_j(\mathbf{K}) \exp(i\, \mathbf{K} \cdot \mathbf{r}_j)$$

If atoms are identical atomic form factors are indep. of j, and S_K reduces to a <u>geometrical</u> structural factor.

Use of conventional unit cells for centered Bravais Lattice is, and should be, equivalent to use of primitive unit cells, because of S_K.

Classification of Bravais Lattice

- Point Group – point is fixed (reflection, rotation, inversion)
- Space Group – point group operations and translations
- 14 Bravais Lattices
  - Cubic – sc, bcc, fcc
  - Tetragonal – simple, centered
  - Orthorombic – simple, base-centered, body-c, face-c
  - Monoclinic – simple, centered
  - Triclinic
  - Trigonal
  - Hexagonal

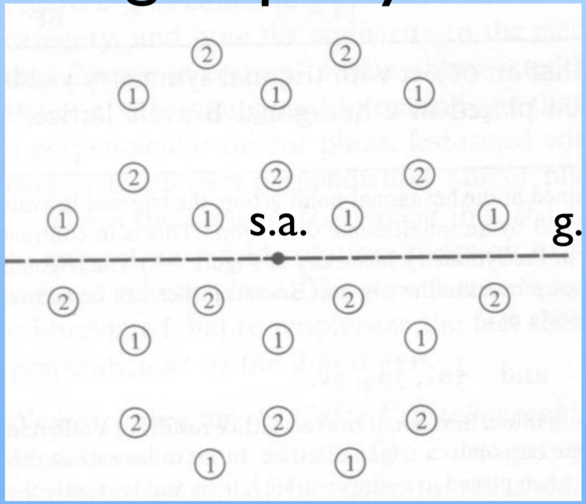
Table 7.1
POINT AND SPACE GROUPS OF BRAVAIS LATTICES AND CRYSTAL STRUCTURES

	BRAVAIS LATTICE (BASIS OF SPHERICAL SYMMETRY)	CRYSTAL STRUCTURE (BASIS OF ARBITRARY SYMMETRY)
Number of point groups:	7 ("the 7 crystal systems")	32 ("the 32 crystallographic point groups")
Number of space groups:	14 ("the 14 Bravais lattices")	230 ("the 230 space groups")

Non-symmorphic space group

- Space group which cannot be considered as a direct product of translation and point group operations is called a "non-symmorphic" group
  - Glide plane (translation + reflection)
  - Screw axis (translation + rotation)

e.g. hcp crystal



230 Space Groups

- General Notations:

  C_n (n; n-fold rot)
  C_{nv} (nmm; v means vertical mirror plane)
  C_{nh} (~ n/m; h means horizontal mirror plane)
  S_n (n-fold rot+reflection, but not each)
  D_n (n22; n-fold rot, 2-fold rot for other axes)
  …

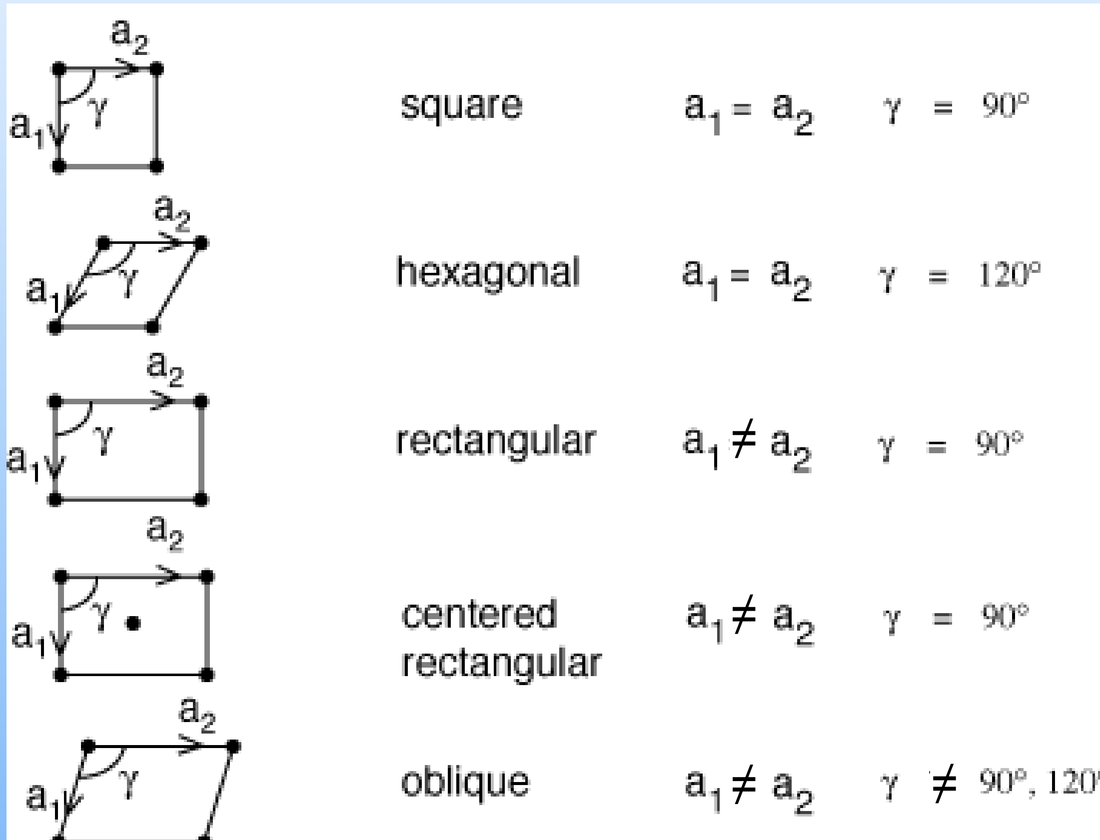
- Best to look it up in books and web sites.

  e.g. http://img.chem.ucl.ac.uk/sgp/mainmenu.htm

  Real crystal struct. data base

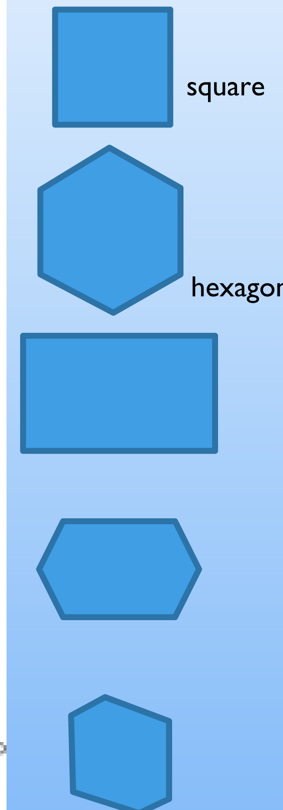
  e.g. http://icsd.ill.fr/icsd/index.html

Classification of Lattice (2d)



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

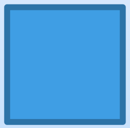
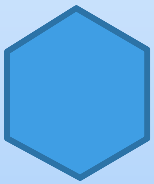
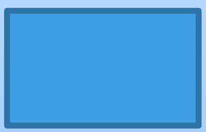
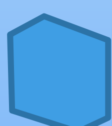
WS Cell Shape



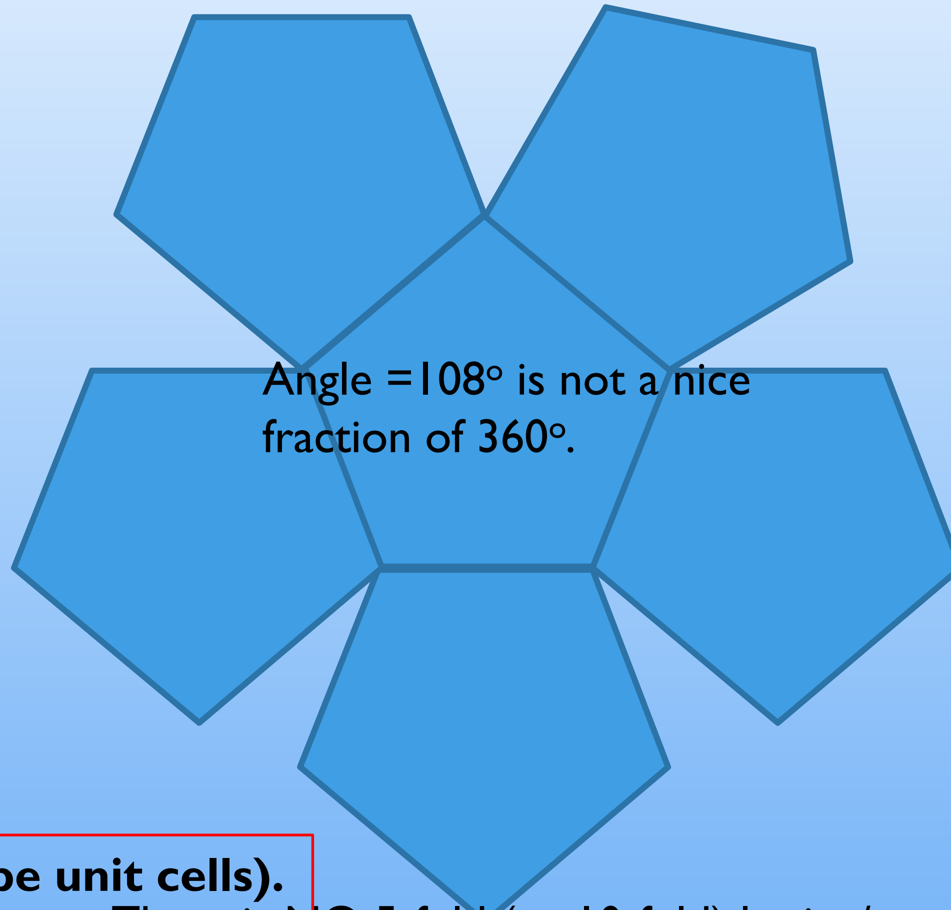
	Symmetry
square	4, v, h, i
hexagonal	6, v, h, i
rectangular	2, v, h, i
centered rectangular	2, v, h, i
oblique	2, i

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

These are <u>all</u> 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.