Classification of Bravais Lattice (BL)

Recall, crystal = lattice + basis
Note that a given lattice can sometimes be expressed as: another lattice + basis

Ex:

First let us consider a basis of a single spherical atom. (isotropic)

Each type of BL is characterised by specification of all rigid operations that takes the lattice on to itself.
Specification of such a set of operation : space group / symmetry group

Rigid opⁿ : Translation by $\vec{R}$
reflection
rotation, inversion.

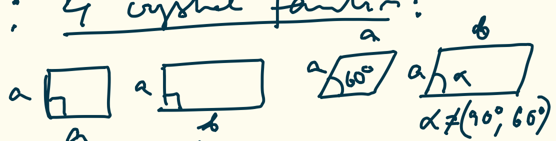
Rigid opⁿ : May or may not keep any lattice pt fixed.
Any sym opⁿ : Translation by $\vec{R}$ + rigid opⁿ that keeps at least one lattice pt fixed.

∴ A full symmetry group : ① Translation through $\vec{R}$
② Opⁿ that leaves a particular pt of lattice fixed.
③ Any opⁿ constructed by successive application of opⁿs ① and ②.

Point group : Subset of full symmetry group : only opⁿs of type ②.
Each pt-group defines one unique family of BLs.
Number of sp. group denotes total number of different types of BLs.

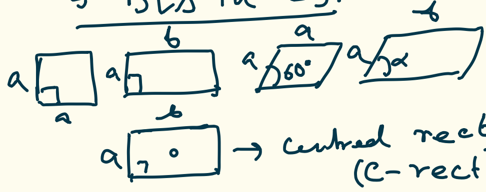
3D : 7 distinct point groups & 14 distinct space groups.
2D : 4 " " " " 5 " " "

Ex in 2D : 4 crystal families :



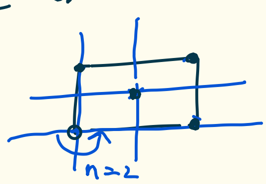
sq. rect. hex. oblique

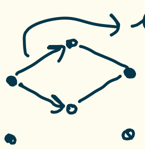
5 BLs in 2D :



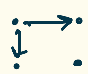
→ centred rect. (c-rect.)

Note the rect. and c-rect. have same symmetries of type ② ⇒ Same pt. Gr.





extra translation symmetry that rect. does not have.



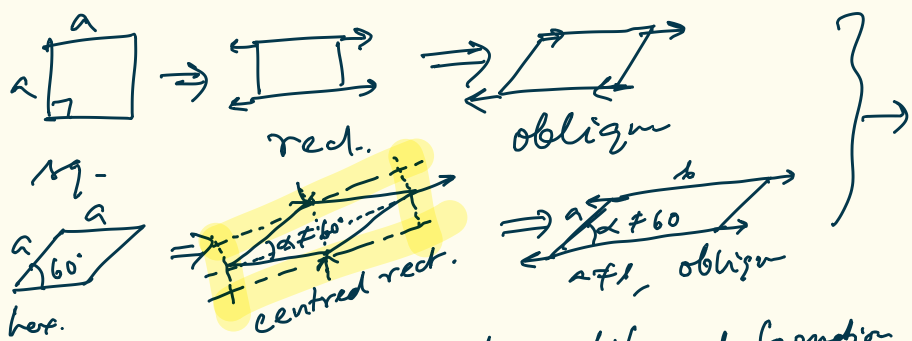
∴ Relaxing the restriction on symm opⁿs to keep at least one lattic pt fixed allows extra translational symmetries which bring more diversity in PUCs.

In 3D : BLs : sc, bcc, fcc in the cubic crystal family.

Bravais Lattice: 7 distinct BL groups in 3D : hierarchy of crystal str.

We start with the BL of highest symmetry and reduce symmetry by appropriately deforming the crystal by arbitrary degree.

2D



Square   hexagonal

↓   ↓

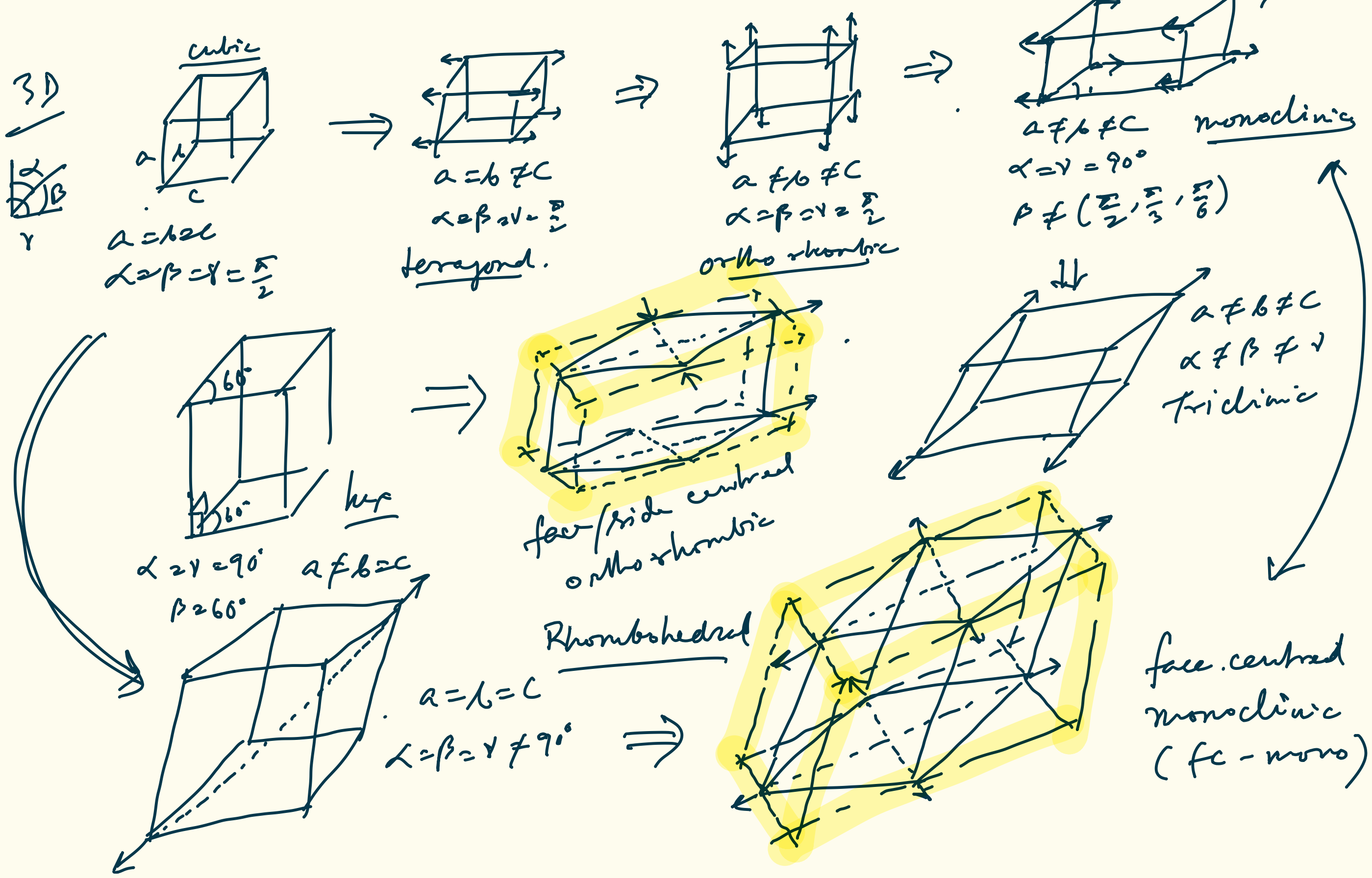
rect, c-rect.

↓

oblique

Note: sq. ⇏ hex by arbitrary deformation

3D



⇒ Cubic → (trigonal) Rhomb. → fc-mono,

Cubic → Tet → Ortho, c-ortho

Hex → Ortho, c-ortho

Ortho, c-ortho → Mono → Triclin.

Note that we can not go from cubic to hex through arbitrary deformation.

Note: So far we have only considered the symmetry of Bravais lattice.

Now let us consider possible shape of basis as well.
If the basis is spherically symmetric then that is the highest symmetric scenario we have already discussed.
Now if the basis also has certain shape of low symmetry then the overall symmetry of the crystal structure will be less than that of the symmetry of the Bravais lattice and thus we will have more variety. ⇒ Actual crystal str (Bravais lattice + basis) has less symmetry and thus more variety than that of the Bravais lattice.

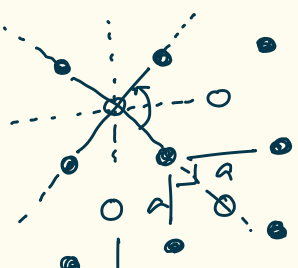
Crystallographic point group : Different than lattice point group.

Rigid point op^n must bring all basis back on to itself across crystal. (ie, Not just the lattice pts)
keep at least one lattice pt fixed).
: Rotation, Reflection, Inversion, Rotation followed by reflection / inversion.
All these operations must happen through points lines or planes passing through lattice points. The lattice points have to be so placed such that the maximum number of fixed point symmetries can be considered through them.

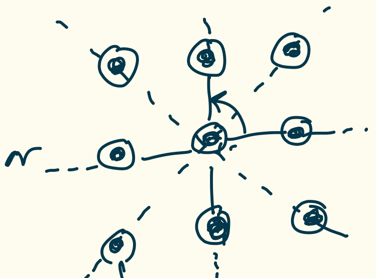
le, Basis atoms : •
lattice points : o

Let us see how to place lattice points to maximize fixed pt. symm operations

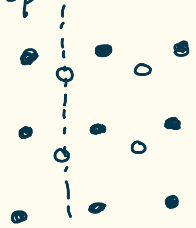
2D



lattice pts exactly in the middle



lattice pt on basis atom (both are equally correct choice)

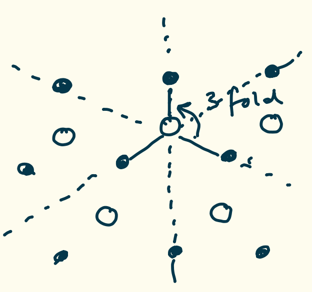


(wrong choice for symmetry analysis)

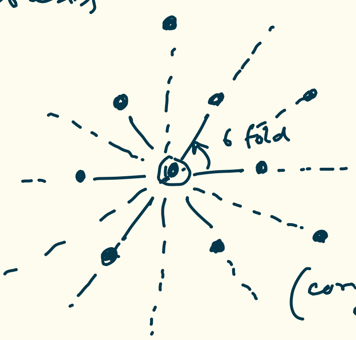
In this choice of lattice only one reflection by mirror at dashed line.

Symm:
1. 4 fold rotational symm
2. Reflection through mirror planes containing the 4 fold axis and intersecting the plane at the dashed lines.
3. Inversion symm

o lattice • basis



3 fold rot^n
Reflection
No inversion
(this choice does not allow all symmetry)



(correct choice)

6 fold rot^n
Reflection
Inversion.

3D

Bravais Lattice (BL)	Crystal structure
(BL + basis of sph. sym)	(BL + basis of arbitrary sym)
7 pt. groups ⇒ 7 crystal family	32 crystallographic pt groups
14 sp. groups ⇒ 14 BLs	230 crystallographic sp. groups

we will restrict to point groups only.

We know: pt group + sym which does not preserve any lattice pt → sp. group

[See fig 7.2   121 for the 5 crys by pt groups of the cubic family
Fig 7.3 page 122 for the non cubic pt groups.]

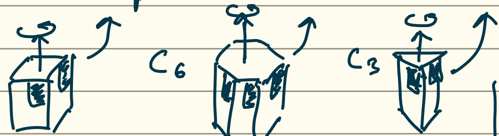
(SCHOENFLIES)

Schoenflies notation of crystallographic pt groups:

Non cubic (we will next extend same to cubic)

Representative blocks having same sym.

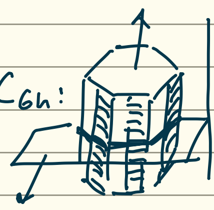
$C_n \rightarrow$ n fold rot^n axis C_4 C_6 C_3



Note that the colour on the faces does not allow any other sym operation like reflection or other rotation

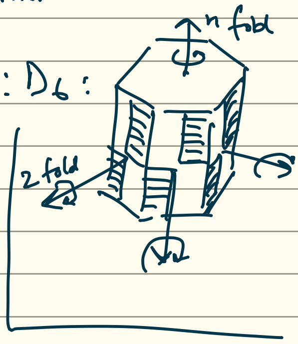
$C_{nv} \rightarrow$ n " " " + mirror (M) containing n fold axis: C_{6v}

$C_{nh} \rightarrow$ n " " " + one M ⊥ to axis: C_{6h}:

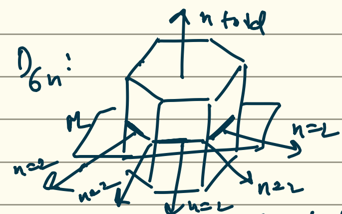


M through dashed line and 6 fold axis.
mirror

$D_n \rightarrow$ n " " " + 2 fold rot^n axis ⊥ to n fold axis: D_6:

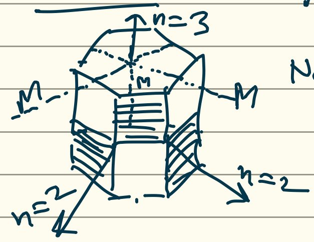


$D_{nh} \rightarrow D_n$ + M ⊥ to n fold axis. D_{6h}:
(Most symmetric)



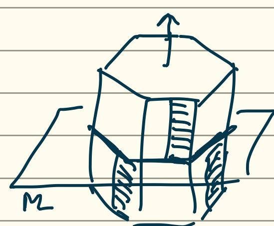
$D_{nd} \rightarrow D_n$ + M containing n fold axis but bisects the angle between 2 fold axis

D_{3d}



Note that this is not D_{6d}
D_{6d} not possible

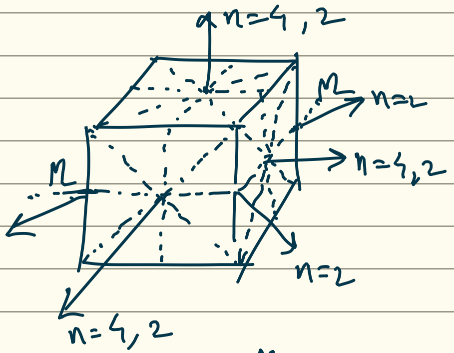
$S_n \rightarrow$ n " rotation-reflection axis S_6:



Apply reflection then rotation.

Cubic crystallographic groups :

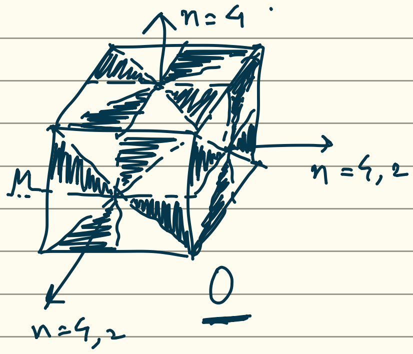
4 fold sym :



----- M

Most symmetric

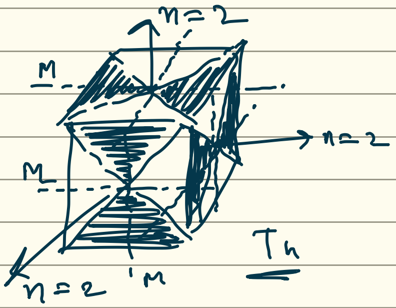
O_h



O

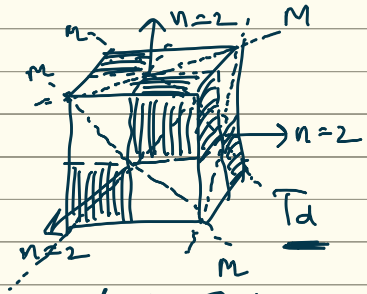
No M plane

2 fold symmetry :



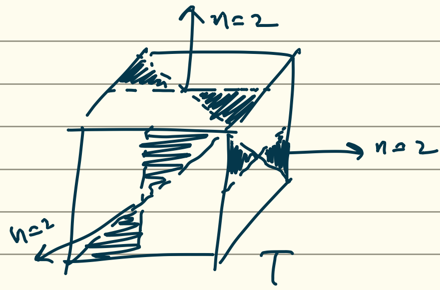
T_h

2 fold rotation
⊥ M plane



T_d

2 fold rotation
Diagonal M plane



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Only 2 fold rotation