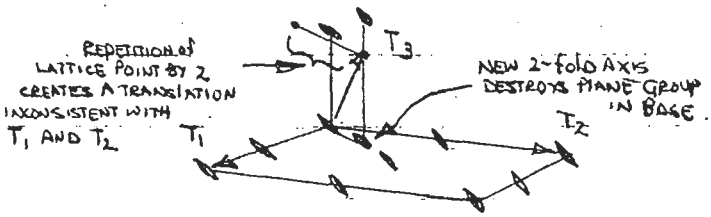
3.60 Symmetry, Structure and Tensor Properties of Materials

DERIVATION OF THE SPACE LATTICES

The point group of a crystal imposes constraints on the lattices with which it may be combined. Specification of a third translation, T_3, which is not coplanar with the pair of conjugate translations T_1 and T_2 which generate a plane net, will define a space lattice. We have seen that the two-dimensional crystallographic point groups (1 2 3 4 6 m 2mm 3m 4mm 6mm) require 5 distinct two-dimensional nets (parallelogram, rectangular, centered-rectangular, square, hexagonal) with which they may be combined to provide 17 two-dimensional plane groups.

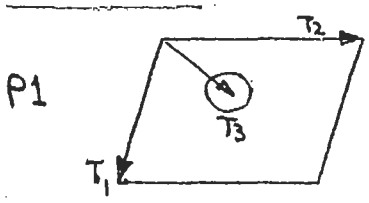
Each of the 5 two-dimensional nets provides a potential base with a distinct "specialness" for a space lattice. However, this "specialness" is present if, and only if, there is symmetry present which requires this "specialness". In a three-dimensional lattice this symmetry cannot be confined just to the two-dimensional base of the cell; it extends through all of space. The constraint imposed on the choice of T_3 to be combined with a two-dimensional net is accordingly, that symmetry elements present in the plane group which requires specialization of the base of the cell must coincide in subsequent layers of the space lattice. For example, if we pick an arbitrary T_3 in combination with plane group P_2, the symmetry of the plane group in the base of the cell is destroyed, and translational periodicity which is incompatible with that of the base is also created.



(The text derives the space lattices by stacking plane nets containing only the rotation axes. Although this leads to the correct results, this procedure is incomplete--all 17 plane groups should be considered. Moreover, the procedure is not rigorous. For example, a two-fold axis by itself in a rectangular net does not require the net to be rectangular: a two-fold axis in a centered-rectangular net permits a choice for T_3 which is impossible when the full plane system is considered.)

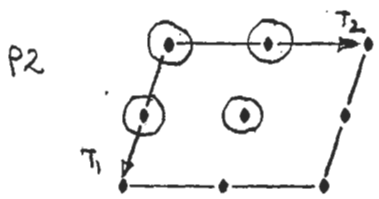
In the following derivation we specify T_3 in terms of 3 components: x (a fraction of T_1), y (a fraction of T_3) and a component z in a direction normal to the plane of the plane group. The possible terminal points of T_3 which make symmetry elements line up are circled in the diagrams. These locations are the independent locations which have the same point group as the origin of the cell.

Point Group 1



T_3: xyz Triclinic Primitive

Point Group 2

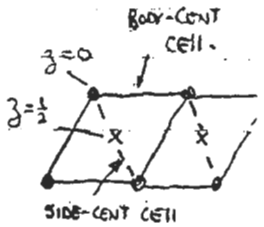


T_3: 00z Monoclinic Primitive

½0z or 0½z Monoclinic Side-Centered

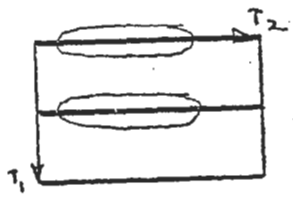
½½z Monoclinic Body-Centered

(Monoclinic side-centered and monoclinic body-centered are not distinct specializations. One may be converted into the other by appropriate redefinition of the parallelogram base, with no loss of specialness.)

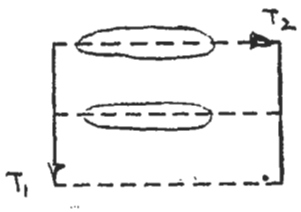


Point Group m

pm



pg



oyz Monoclinic Primitive

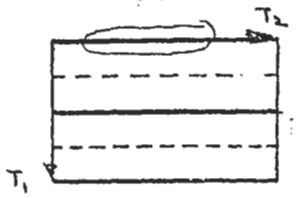
(As above, except here "base" of cell is one of the rectangular faces; parallelogram face contains T_2 and T_3)

½yz Monoclinic Body-Centered

(or side-centered)

Point Group m

cm

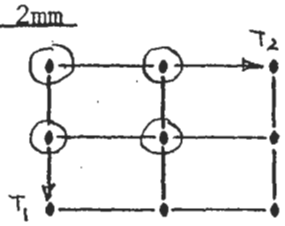


oyz Monoclinic Side-Centered

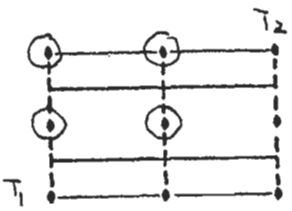
(Note that ½yz is no longer distinct--a lattice point exists on both the mirror plane at x = 0 and the mirror plane at x = ½. The mirror planes are not independent as in pm.)

Point Group 2mm

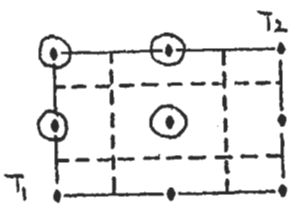
P2mm



P2mg



P2gg



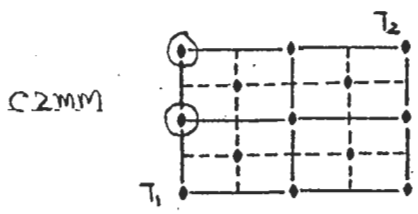
ooz Orthorhombic Primitive

½oz and o½z Orthorhombic Side-Centered

½½z Orthorhombic Body-Centered

(Note that here, unlike the monoclinic system, both the side-centered and the body-centered lattices are distinct. One cannot transform one into the other without degrading the rectangular base to a parallelogram and losing specialization.)

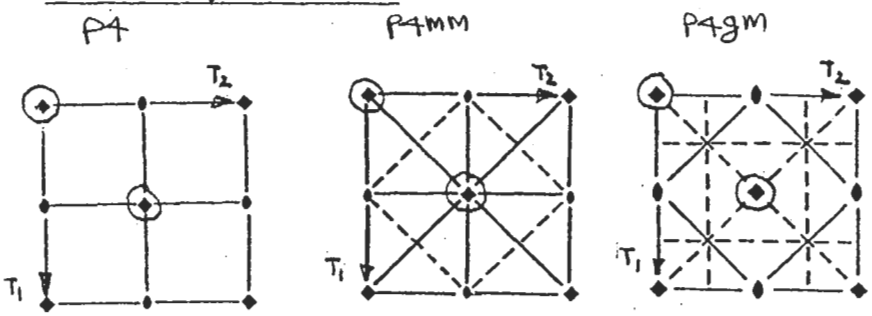
Point Group 2mm



ooz Orthorhombic Primitive (Note that $\frac{1}{2}\frac{1}{2}z$ is now the same as this choice: lattice points exist in the base at both 00 and $\frac{1}{2}\frac{1}{2}$. Both lead to lattice points directly over one another in subsequent nets in the stack.)

$\frac{1}{2}$oz Orthorhombic Face-Centered (Note that o$\frac{1}{2}$z is now equivalent to this choice. Both are points of 2mm symmetry displaced from a lattice point by $\frac{1}{2}\vec{T}_1$.)

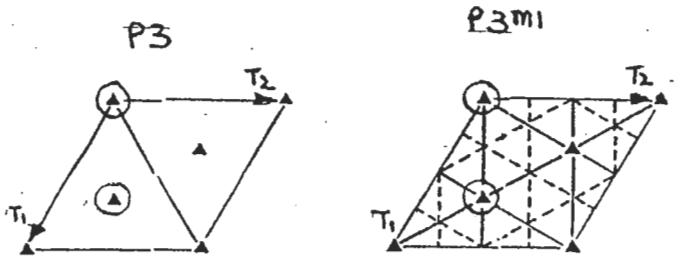
Point Groups 4 and 4mm



ooz Tetragonal Primitive

$\frac{1}{2}\frac{1}{2}z$ Tetragonal Body-Centered

Point Groups 3 and 3m

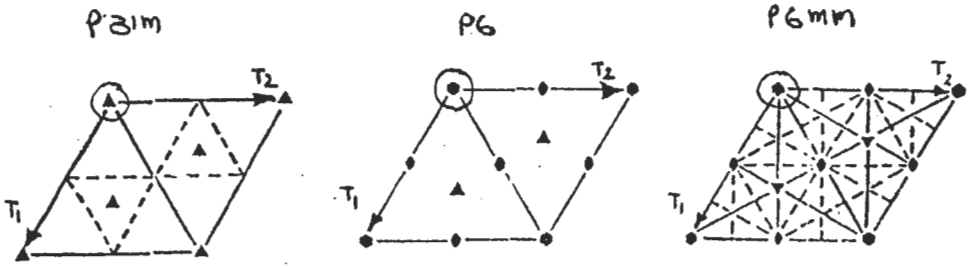


ooz Hexagonal Primitive

$\frac{2}{3}\frac{1}{3}z$ Hexagonal Rhombohedral

(Note: the third 3-fold axis at $\frac{1}{3}\frac{2}{3}$ is an independent symmetry element in this case, but the choice of $\frac{1}{3}\frac{2}{3}z$ for T_3 does not lead to a distinct lattice. Upon rotating the lattices to the left by 180° this choice will be seen to give the same result.)

Point Groups 3m (alternate setting), 6 and 6mm



ooz Hexagonal Primitive

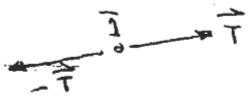
(Note that the choice of $\frac{1}{3}\frac{2}{3}z$ or $\frac{2}{3}\frac{1}{3}z$ is here impossible. Different symmetry exists at these locations than at the origin.)

The stackings of the 17 plane groups considered above have provided 11 distinct space lattices (it is amusing to note, also, that by so doing we have obtained 32 of the 230 three-dimensional space groups). These are the space lattices required by only 10 of the 32 three-dimensional point groups (namely, those which are also two-dimensional in nature).

We next examine the additional requirements, if any, imposed on space lattices by the remaining 32-10=22 point groups.

1. The requirements of point groups C_n (1, 2, 3, 4, 6) and C_{nv} (2mm, 3m, 4mm and 6mm) have been obtained above by stacking the plane groups.

2. Requirements of $\bar{1}$: The presence of $\bar{1}$ in a lattice requires that for every translation $\vec{T}$ a translation $-\vec{T}$ must exist. This is true of any lattice, so $\bar{1}$ requires only the general triclinic primitive lattice.



*The fact that inversion imposes no restriction on a lattice now permits us to use symmetry arguments to shorten the list of point groups which need to be considered further. If inversion imposes no restriction, then any point groups which become the same upon addition of inversion must require the same constraints of the lattice.

e.g.: $2 + \bar{1} = 2/m$. $\bar{1}$ imposes no constraint, so lattices required by 2/m must be identical to those required by 2. (i.e., monoclinic)

Therefore, in deriving the remaining space lattices we need to consider the requirements of the 11 Laue Groups--or, better yet, any simpler representative point group in the collection which becomes the Laue Group upon the addition of inversion.

e.g.: 222, 2mm and 2/m 2/m 2/m all become the Laue Group 2/m 2/m 2/m upon addition of $\bar{1}$. Therefore all require the same lattice types. Rather than consider the higher symmetry of the Laue Group itself, we can instead work with a simpler symmetry such as 222 or 2mm.

Point Groups Already Considered by Stacking Plane Groups	Resulting Lattice Types	Other Point Groups Which Correspond to the Same Laue Group
1	Triclinic Primitive	$\bar{1}$
2,m	Monoclinic Primitive Monoclinic {Side-Centered Body-Centered	2/m
2mm	Orthorhombic Primitive Side-Centered Body-Centered Face-Centered	222, 2/m 2/m 2/m

Point Groups Already Considered by Stacking Plane Groups	Resulting Lattice Types	Other Point Groups Which Correspond to the Same Laue Group
4 4mm	Tetragonal Primitive Body-Centered	$\bar{4}$, 4/m 422, $\bar{4}$2m, 4/m 2/m 2/m
3 3ml	Hexagonal Primitive or Rhombohedral	$\bar{3}$ 312,$\bar{3}$ 2/m
31m 6 6mm	Hexagonal Primitive	321,$\bar{3}$ 2/m 3/m,6/m 622,$\bar{6}$ 2/m,6/m 2/m 2/m

Using this neat device, one sees that the requirements of all remaining 32 - 10 = 22 point groups have been treated with the exception of the cubic point groups.

If you do not like this shortcut, one can deal with the point groups in the right-hand column on a case-by-case basis.

Example: Point group 4 requires tetragonal primitive or body-centered. 4/m has an additional horizontal m. m requires that a rectangular (or centered rectangular) net be normal to it. This is automatically satisfied by the rectangular sides of the tetragonal lattices.

422 has additional two-fold axes normal to 4. 2 requires only that a parallelogram net be normal to it. The requirements of 2 are thus satisfied if we orient 422 in the tetragonal cells such that the two-fold axes are normal to the rectangular sides of the cell. (The two-fold axes 45° away from the sides of the cell find themselves normal to (110), which is also a rectangular net, and thus are also perfectly happy.) Thus 422 may be accommodated in either of the two tetragonal cells.

Requirements of Cubic Point Groups

Laue Group: 4/m $\bar{3}$ 2/m corresponding point groups: 432,$\bar{4}$3m,4/m $\bar{3}$ 2/m

Laue Group: 2/m $\bar{3}$ corresponding point groups: 23, 2/m $\bar{3}$

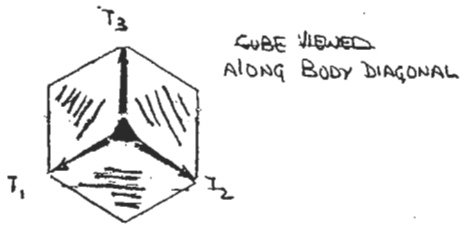
Consider, for simplicity, the two simplest axial arrangements. The others must have the same requirements.

Point Group 23

Start with the three orthogonal two-fold axes. This requires, at minimum, one of the orthogonal brick-shaped orthorhombic cells of 222.

i.e., Primitive
Side-Centered
Body-Centered
Face-Centered

The three-fold axes must be oriented along the body-diagonals and, by rotation, require that the three cell edges be equal.

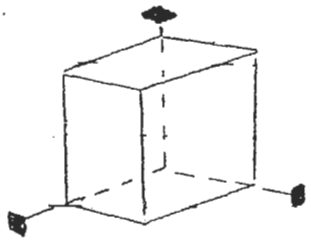


This leads to Primitive Cubic
Body-Centered Cubic
Face-Centered Cubic

(The side-centered orthorhombic cell also leads to the face-centered cubic lattice as the three-fold axis requires that all faces of the cube be equivalent. Each must accordingly bear a centered lattice point.)

Point Group 432

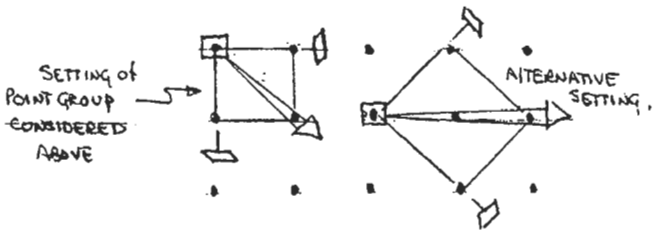
Start with the tetragonal primitive and body-centered cells which, at minimum, are required by one four-fold axis.



The two additional orthogonal four-fold axes now require that all faces of the cell be square and, as above, the three-fold axis requires that all edges and faces be equivalent. The tetragonal P and I lattices thus become

Primitive Cubic
Body-Centered Cubic

At first glance it appears as though 432 does not require a face-centered cubic lattice. There is, however, an alternate setting possible for 432 relative to the tetragonal lattices considered above. Note that the square base of the cell may be redefined as a centered double net which is also square. (The primitive tetragonal lattice thereby becoming base-centered, the body-centered tetragonal lattice becoming face-centered). It may now be readily appreciated that the four-fold axes may also be oriented normal to the faces of these redundant multiple cells, and the three-fold axes along the body diagonal. As above, symmetry requires the lattices to become cubic with all faces equivalent. Both tetragonal lattices thus become Face-Centered Cubic for this point group setting.



There are thus 14 unique space lattices.