3.60 Symmetry, Structure and Tensor Properties of Materials

Principles of Plane Group Derivation

(Note: this material is not treated in the text!)

① Summary of Principles in Advance (that is, an Abstract)

(a) Add each of the two-dimensional point groups to each of the two-dimensional lattice nets which can accomodate them. Each of the operations of the point group combined with each of the independent lattice translations which terminates within the unit cell must create some new symmetry operation elsewhere within the cell. Locate these using the "combination theorems", expressions in an algebra of operations that specify the net effect of two sequential symmetry tranformations

$$T_{\perp} \cdot A_{\alpha} = B_{\alpha} \;@\; \frac{T_{\perp}}{2} \cot \frac{\alpha}{2}$$

$$T \cdot \sigma_{\tau} = \sigma'_{\tau + T_{\parallel}} \;@\; \frac{1}{2} T_{\perp}$$

(b) Symmetry planes in a point group must be mirror planes, but glides are permitted in a plane group as it is translationally periodic. Replace, therefore, each of the pure mirror planes in the point groups of (a) by glides, and locate the additional symmetry elements which arise using the above combination theorems

(c) Symmetry planes and axes need no longer intersect in a plane group. Therefore, starting with the plane groups which consist of rotation axes (alone) placed in a plane net, attempt to interleave glide planes or mirror planes with the axes in such a way that no new axes are created. For each possible combination find the new symmetry elements which arise using the above combination theorems and the new theorem:

$$\boxed{\sigma_{\tau} \underbrace{\cdot}_{\delta} A_{\pi} \underbrace{=}_{\tau/2} \sigma'_{2\delta}}$$

② The Two-Dimensional Lattices (Nets)

Earlier we had shown that rotation and reflection require 5 types of two-dimensional lattices, each with a distinct sort of specialization which is dictated by symmetry

1-fold or 2-fold axis: Parallegram net
4-fold axis: Square net
3-fold or 6-fold axis: Equilateral (or hexagonal) net
Mirror plane: Either a primitive or centered (diamond) rectangular net

③ The Two-Dimensional Point Groups

Let's now ask how one can combine, about a fixed point in space, more than one of the two-dimension symmetry elements which can subsequently be combined with a two-dimensional lattice net — namely, 1, 2, 3, 4, 6 and m. A ground rule that we will impose is that all mappings of coordinates that occur must involve only the two dimensions of the space. We will not allow an operation that lifts a motif out into a third dimension and then restores it to the two-dimensional space of our plane (any more than we would entertain an operation in three dimensions that plucks things out into a forth dimension and then pops them subsequently back into three!)

The single symmetry elements that meet this restriction are

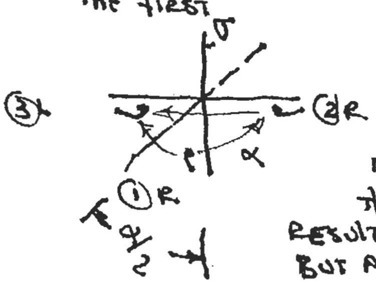
(a) A rotation axis (normal to the plane of the 2-D space) which maps things only within the plane normal to the axis

(b) A mirror plane (normal to the plane of the 2-D space) which maps things left-to-right across the mirror line.

If rotation axes and mirror lines, separately, act as 2-dimensional symmetry elements that leave at least one point in space invariant, they will clearly do so in combination, <u>provided</u> they intersect at a point (which will be the locus that is left invariant).

If we combine two operations, however, we will (like it or not!) introduce a third operation into the space. We will thus need another "combination theorem" that will, once and for all, specify the result.

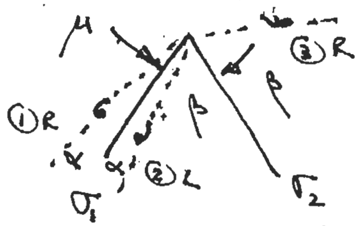
(a) The combination of a rotation A_α with a reflection σ about a locus passing through A is equivalent to a new reflection operation σ' about a locus $\alpha/2$ from the first



Note that the initial pair of operations does <u>not</u> commute! Change the order and the result is again reflection but across a different location — $\alpha/2$ on the <u>other</u> side of the initial reflection locus

$$\boxed{\underbrace{\sigma \cdot A_\alpha = \sigma'}_{\alpha/2}}$$

(b) The combination of two successive reflection across loci that intersect at a point



Let the angle between σ_1 and σ_2 be defined as μ. The successive reflection produce a third motif of the same handedness — ∴ the net transformation must be <u>rotation</u>. The amount of rotation is $(\alpha + \alpha + \beta + \beta)$ but $\alpha + \beta = \mu$ thus

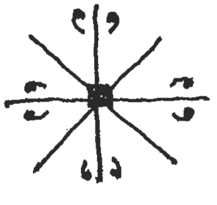
$$\boxed{\underbrace{\sigma_2 \cdot \sigma_1}_{\mu} = A_{2\mu}}$$

The pair of reflection operations does not commute either. Change the order and the result is $A_{-2\mu}$

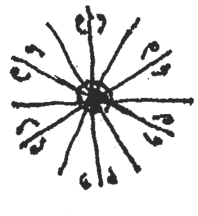
The new symmetry combinations that result from application of either of these theorems are

2mm

3m



4mm



6mm

It is convenient to have a symbol for each of the possible combinations. There are, in fact two!

The <u>International Symbol</u> is a running list of the <u>independent</u> symmetry elements that are present. ("Independent" means not related to another by some other symmetry element. "Independent" symmetry elements are also "different" in the way in which motifs are hung on them) Note that in "4mm", for example, the mirror lines that are 45° from the adjacent mirror lines are not related by the 90° rotation of the 4-fold axis. The also differ in the way the closest pair of motifs are arranged — different distance from the mirror and facing in a distinct direction.

Thus the combination of 4 with a mirror plane leads to <u>4mm</u> (convenient, concise — if we listed <u>all</u> of the mirrors that were present it would be "4mmmmmmmmm" quite a mouthful !!)

Note that the combination of a 3-fold axis is different in this respect: there is only <u>one</u> independent mirror and the symbol used is thus <u>3m</u>

The <u>Schönflies symbol</u> (after one of the three investigators who independently and almost simultaneously derived the 3-D space groups) is based on group theory. "C" was used to denote a "cyclic group", defined as one in which all elements are "powers" of a basic operation. (For example, 4 contains $\left\{ \underset{90^\circ}{A_{\frac{\pi}{2}}} \; \underset{180^\circ}{A^{2}_{\frac{\pi}{2}}} \; \underset{270^\circ}{A^{3}_{\pi/2}} \; \underset{360^\circ}{A^{4}_{\frac{\pi}{2}}} \right\}$ as elements. The rank of axis is apended as a subscript. Thus C_4 for a 4-fold axis. Addition of a "vertical" (in anticipation of the three-dimensional analog) mirror plane is indicated by a "v" appended to the subscript. m is denoted by "C_s" (it is a cyclic group and the "s" represents "Spiegel" — mirror in German)

The two dimensional crystallographic point groups are thus

1	2	3	4	6	m	2mm	3m	4mm	6mm
C_1	C_2	C_3	C_4	C_6	C_s	C_{2v}	C_{3v}	C_{4v}	C_{6v}

They are termed <u>Point Groups</u> because the operations (elements) in each conform to the postulates of the mathematical entity defined as a "group" and these operations leave at least one point in space invariant. The qualifier "crystallographic" is required becauses these are the only point groups that one can combine with a lattice. (The point groups 8mm or 5m are quite lovely, but one could never find them in a crystal)

(Note some consequences of the ground rules which have established in defining these two-dimensional point groups:

<u>There is no inversion center in two dimensional patterns</u>

In 3-D the mapping of a 2-fold axis parallel to z is $xyz \rightarrow \bar{x}\bar{y}z$

that of an inversion center is $xyz \rightarrow \bar{x}\bar{y}\bar{z}$

} These are indistinguishable if there is no z coordinate!

<u>There can be no 2-fold axes lying in the plane of the pattern</u>

This operation would lift the pattern out into three dimensions and restore it to the two-dimensional space "upside down" — which is not defined in a strictly two-dimensional space.

One <u>could</u> derive symmetries in which these operations were included, and this in fact would lead to something called the "two-sided plane groups" (eg, a sheet of paper with pattern on <u>both</u> surfaces) — but these are different bersis!)

④ Distribution of 2-Dimensional Point Groups among the 2-Dimensional Lattices

The 2-D nets required by a pure rotation axis or a pure mirror plane are given above in ②. We now ask whether the 2-D point groups of the type C_{nv} require any new types of nets with distinct sorts of specialization.

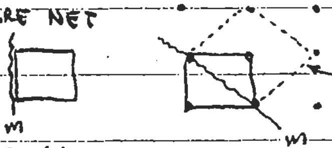
2mm — Each m requires the net to be rectangular (primitive or centered)

The 2-fold axis requires <u>no</u> specialization

∴ <u>2mm requires either of the rectangular nets required by m</u>

4mm — The 4-fold axis requires that the net be square

The two m's require that they be along the edge of a primitive or centered rectangular net. This specialization is included in that incorpated in a square net



Double cell ≡ centered square (also a centered rectangle)

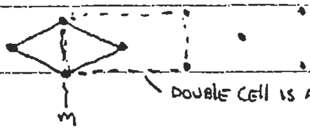
∴ 4mm requires only the square net of 4

3m & 6mm — The 3-fold axis or 6-fold axis requires an equilateral net

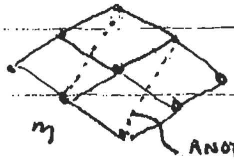
<u>The m's must be along the edge of a primitive or centered rectangular net</u>

This specialization is already included in the equilateral net as it is a special case of a diamond net

∴ 3m or 6mm requires only <u>the equilateral net of 3 or 6</u>



Double cell is a centered rectangle.



Another choice for a centered rectangle

~~For future reference~~

Note that there are thus two allowable settings for a mirror plane in a hexagonal net: along the edge of the cell <u>or</u> normal to the edge of the cell

The final distribution of the 10 2-dimensional point groups among the 5 2-dimensional lattices is thus

Point Groups (10)	Lattice Types (5)
1 2	Parallelogram
m 2mm	Primitive Rectangle or Centered Rectangle (Diamond)
4 4mm	Square
3 6 3m 6mm	Equilateral

⑤ DERIVATION OF THE PLANE GROUPS

5.1 DIRECT ADDITION OF A POINT GROUP TO A LATTICE TYPE

Twelve potential plane groups result from the direct addition of the 10 point groups in the table above to the lattice points of the nets which can accomodate them. As a symbol used to designate each result we will use a notation which consists of two parts; a first symbol to designate the lattice type, and a second part to designate the point group or symmetry which has been added to the lattice point

Thus; for example:

A parallelogram net + point group 2 added to a lattice point = plane group p2

We need not, in the symbol for the plane group, specify that the lattice is a parallelogram. (The p stands for primitive) As the informed reader is aware that point group 2 requires only that the lattice be an unspecialized parallelogram. Thus the only two symbols which appear for lattice types in the symbols for the plane groups are p (for primitive) and c (for centered) and, moreover, the latter is needed only for the case of the two rectangular nets.

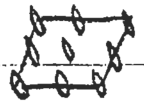
Eventually we will derive three-dimensional space groups for which similar symbols will be used. There is, accordingly, some scope for ambiguity: we might, for example, add symmetry 1 to a primitive, general two-dimensional net here, and later add 1 to a primitive, general three-dimensional space lattice. To distinguish 3-D space groups from 2-D plane group symbols, an upper-case letter is useds for the lattice type of the former, a lower-case letter for the lattice type of the latter

Thus P1 ⇒ 3-D space group
p1 ⇒ 2-D plane group

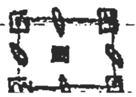
ADDITION OF A ROTATION AXIS TO A NET

Parallelogram net + 1 = $\boxed{p1}$

Parallelogram net + 2 = $\boxed{p2}$

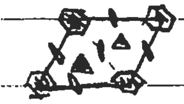


Square net + 4 = $\boxed{p4}$



∴ Equilateral net + 3 = $\boxed{P3}$

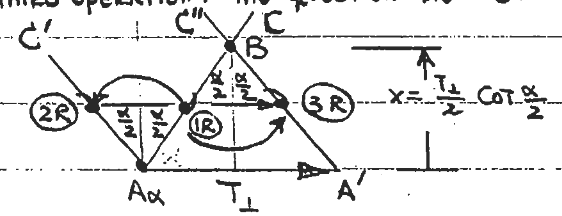
Equilateral net + 6 = $\boxed{P6}$



Combination Theorem:

In each of the above cases we have added a group of rotation operations to a lattice translation which is perpendicular to the rotation axis. As always, the combination of two operations in a space must create the presence of a third operation. The question then is:

$$T_\perp \cdot A_\alpha = ?$$



In the construction to the left

① Combine operation A_α with a translation $T_\perp$ which is perpendicular to it

② Construct a line AC which makes an angle $\frac{\alpha}{2}$ with the perpendicular to the plane of A and $T_\perp$

③ The action of A_α maps line AC to a new line AC′ $\frac{\alpha}{2}$ on the other side of the perpendicular (taking, for example, an object ① which is right handed, say, to object ②, also right-handed

(Note that this is a special case and we will eventually, when working with space lattices, have to consider the case where the translation is NOT perpendicular to the rotation axis)

④ The translation $T_\perp$ maps line AC′ to A′C″ (and object ②R to ③R)

⑤ How is ① related to ③? Not by reflection, as this changes the "handedness" of the object. Not by translation, as the separation between ① and ③ depends on the location along AC where the initial object is placed. That leaves only rotation. The location of a rotation axis is the locus of points left unmoved by that operation; the only point along AC which is unmoved is point B, at the intersection of AC and A′C″, and this point may be seen to be located a distance $x = \frac{T_\perp}{2} \cot\frac{\alpha}{2}$ along the perpendicular bisector of $T_\perp$. Note, also, that the angular throw of rotation axis B is also α, and in the same sense as A_α.

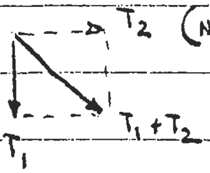
$$\therefore \boxed{T_\perp \cdot A_\alpha = B_\alpha \ @ \ \frac{T_\perp}{2} \cot\frac{\alpha}{2} \text{ along } \perp\text{-bisector of } T_\perp}$$

This theorem was used to derive the location of the additional rotation axes which are depicted above in plane groups P1 through P6. To do so, we combine each of the individual rotation operations implied by the presence of the rotation axis with each of the independent translations within the unit cell (there are an infinite number of translations in a lattice, but the nature of a plane group is fully characterized by the contents of a unit cell; combination of a rotation operation with a very long translation to a lattice point far outside the cell will obviously create a rotation operation which is also far outside the cell and which must be translation-equivalent to one within the cell)

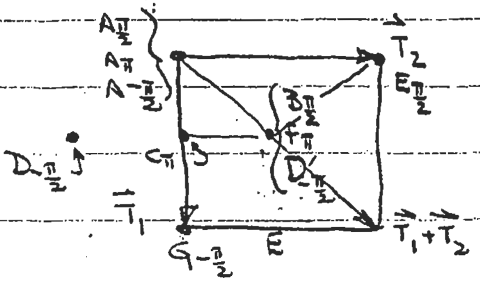
As an example we derive P4:

4 +

$$= \left.\begin{matrix} A_{\frac{\pi}{2}} \\ A_{\pi} \\ A_{-\frac{\pi}{2}} \end{matrix}\right\} + \left\{\begin{matrix} T_1 \\ T_1+T_2 \end{matrix}\right.$$



(Note that T_2 is symmetry-equivalent to T_1 by the 4-fold axis and need not be separately considered)

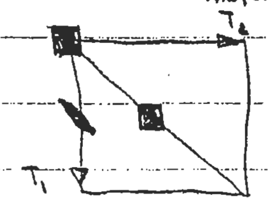


$$\begin{cases} T_1 \cdot A_{\frac{\pi}{2}} = B_{\frac{\pi}{2}} @ \frac{T_1}{2} \cot 45^\circ = \frac{T_1}{2} \\ T_1 \cdot A_{\pi} = C_{\pi} @ \frac{T_1}{2} \cot 90^\circ = 0 \\ T_1 \cdot A_{-\frac{\pi}{2}} = D_{-\frac{\pi}{2}} @ \frac{T_1}{2} \cot -45^\circ = -\frac{T_1}{2} \equiv D'_{-\frac{\pi}{2}} \text{ (REPEATED BY } T_2) \end{cases}$$

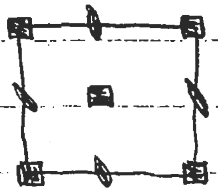
$$\begin{cases} (\vec{T}_1+T_2)\cdot A_{\frac{\pi}{2}} = E_{\frac{\pi}{2}} @ \frac{|\vec{T}_1+\vec{T}_2|}{2} \cot 45^\circ = \frac{1}{2}|(\vec{T}_1+\vec{T}_2)| \\ (\vec{T}_1+\vec{T}_2)\cdot A_{\pi} = F_{\pi} @ \frac{|\vec{T}_1+\vec{T}_2|}{2} \cot 90^\circ = 0 \\ (\vec{T}_1+\vec{T}_2)\cdot A_{-\frac{\pi}{2}} = G_{-\frac{\pi}{2}} @ \frac{|\vec{T}_1+\vec{T}_2|}{2} \cot -45^\circ = -\frac{1}{2}|\vec{T}_1+\vec{T}_2| \end{cases}$$

thus we have $\left.\begin{matrix} B_{\frac{\pi}{2}} \\ F_{\pi} \\ D_{-\frac{\pi}{2}} \end{matrix}\right\}$ All operations of 4-fold axis at center of cell

C_{π} } All operations of a 2-fold axis at midpoint of edge of cell



Repetition of these axes by translation and rotation ⟹



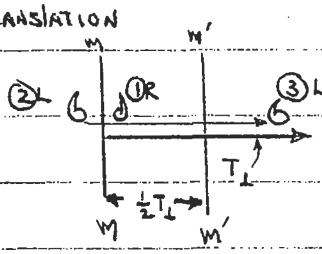
Note that the 4-fold axis at the center of the cell is independent and not symmetrically-related to the 4-fold axis at the origin.
All 2-fold axes are, however, equivalent

(The other combinations of a rotation axis with a net are derived in detail in the text, pp 72-79)

ADDITION OF A MIRROR PLANE TO A NET

Combination theorems: we derived the primitive rectangular net by adding a mirror plane normal to a translation

$T_\perp \cdot m = ?$

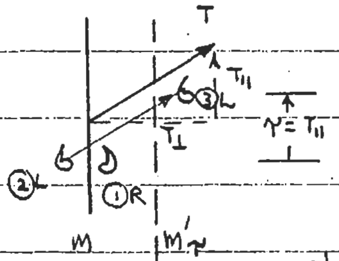


①R and ③L are directly related by a new mirror plane m', parallel to the first and at a distance $\frac{1}{2}T_\perp$ from the first.

Thus $\boxed{T_\perp \cdot m = m' @ \tfrac{1}{2}T_\perp}$

Suppose now that the combination is more general and the translation is no longer exactly perpendicular to the mirror plane but instead has a component $T_\perp$ which is normal to the mirror plane and a component $T_{\parallel}$ which is parallel

$T \cdot m = ?$

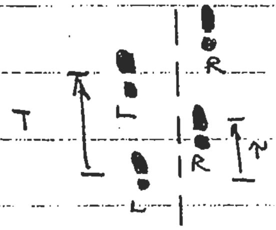


①R and ③L must be related by reflection in some way as their "handedness" differs, but ③ is not directly across from ① and instead is slid along parallel to the orientation of the original plane by an amount $T_{\parallel}$

There is no way in which we can use one of our basic operations to specify the relation between ① & ③. They are related by an operation which contains two separate steps — reflection in a new plane (halfway along $T_\perp$ as before) followed by translation by an amount $T_{\parallel}$. This is a new two-step symmetry operation which (as in the case of $\bar{4}$) simply cannot be described any more directly. The symmetry element is called a glide plane, and an individual operation is designated m_γ, where γ is the translation component

$\boxed{T \cdot m = m'_\gamma @ \tfrac{1}{2}T_\perp}$

Characteristics of Glide: The pattern produced by a glide consists of alternating left and right-handed objects on either side of a planar locus, and separated by a translation component τ.



The symbol for an individual operation is m_τ

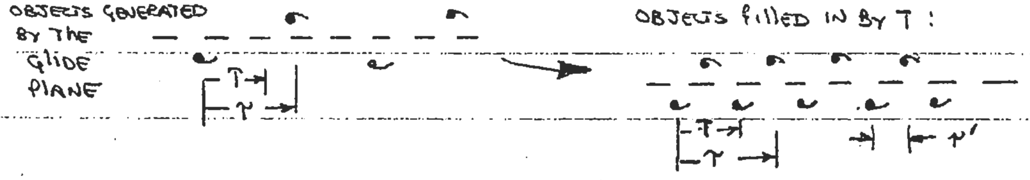
The symbol for the symmetry element itself is g in two dimensions (in three dimensions we will subsequently adopt a notation which specifies the orientation of τ relative to the cell edges)

The symbol for denoting the locus of a glide plane (viewed edge-on and normal to τ) in a pattern is a dashed line (as opposed to a bold, solid line for m)

Note that performing the glide operation twice produces a third object which is translation-equivalent to the first. That is, $m_\tau^2 = T$. A consequence of this is that glide can only appear in a pattern which is translationally periodic in at least one dimension.

From the above, $T = 2\tau$. Or, conversely, turning this around, $\tau = \frac{1}{2}T$. Thus if we attempt to add a glide plane to a lattice, τ for a glide plane must be parallel to some translation in the lattice, and τ must be equal in magnitude to one-half of that translation. Upon adding a glide plane to a lattice, therefore, we are specifying both T and τ. Let us examine the nature of the pattern produced if we specify some τ larger than $\frac{1}{2}T$ (τ must still however be related to T as performing the glide operation twice is equivalent to translation. All that is strictly required, though, is that 2τ be an integral multiple of T)

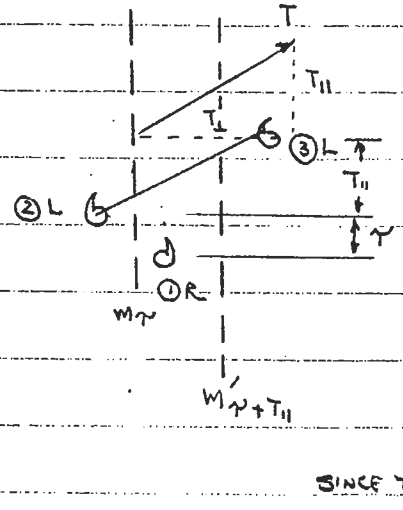
Assume, for example that $\tau = \frac{3}{2}T$ (with $m_\tau^2 = 3T$)



Note that this pattern is indistinguishable from one which would be generated with $\tau' = \frac{1}{2}T$

Thus, while it may be useful to specify a relation between a particular pair of objects by a glide operation with $\tau > \frac{1}{2}T$ (one, for example, may arise as the result of application of a combination theorem), the value of τ for a glide plane may always be redefined by the addition or subtraction of an integral number of translations such that τ is always either 0 or $\frac{1}{2}T$

Most general theorem for combination of a symmetry plane with a translation: The two theorems on pg ⑤ may be generalized to the ~~most~~ general case — combination of a glide plane with a translation inclined to it



Object ① is now related to ③ directly by a new plane, parallel to the first and located $\frac{1}{2}T_{\parallel}$ away (as before), and with a glide translation-component equal to the sum of τ of the original glide plus $T_{\parallel}$

ie,

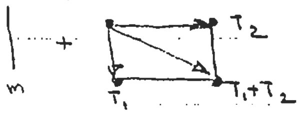
$$\boxed{T \cdot m_\tau = m'_{\tau+T_{\parallel}} \ @ \ \tfrac{1}{2}T_{\perp}}$$

Note that all preceding theorems of this family are special cases of this result with τ and/or $T_{\parallel}$ equal to zero

Since the new glide component, τ', is equal to $\tau + T_{\parallel}$ we may have to subtract of an integral translation to establish whether the new plane is a mirror or gl

HAVING OBTAINED THE THEOREMS NECESSARY TO DEDUCE THE NEW SYMMETRY ELEMENTS WHICH ARISE WHEN A MIRROR PLANE OR GLIDE PLANE IS COMBINED WITH TRANSLATION, LET'S CONTINUE WITH DERIVATION OF THE PLANE GROUPS WHICH RESULT FROM DIRECT ADDITION OF A POINT GROUP TO A LATTICE POINT

m + PRIMITIVE RECTAGULAR NET



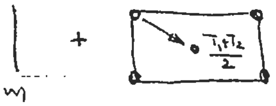
$T_1 \cdot m = m'_{T_1} \equiv m'$ @ 0 ALONG ⊥ (ie, ON TOP OF ORIGINAL m NOTHING NEW)

$T_2 \cdot m = m'$ @ $\frac{1}{2}$ ALONG T_2 THIS IS A NEW m THROUGH THE CENTER OF THE CELL

$(T_1+T_2) \cdot m = m'_{T_1} \equiv m'$ @ $\frac{1}{2} T_2$ SAME AS THE ABOVE MIRROR PLANE

$\boxed{Pm}$

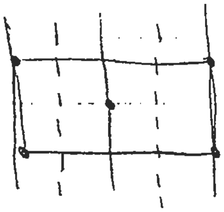
m + CENTERED RECTAGULAR NET



CONTAINS ALL OF THE OPERATIONS ABOVE FOR Pm PLUS

THE ADDITIONAL TRANSLATION $\frac{\vec{T}_1+\vec{T}_2}{2}$ TO THE CENTERED LATTICE POINT

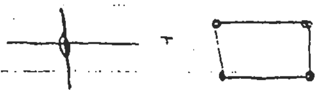
$\left(\frac{T_1+T_2}{2}\right) \cdot m = m'_{\frac{T_1}{2}}$ @ $\frac{1}{2} \cdot \frac{1}{2} T_2$ THIS IS A NEW GLIDE PLANE WITH $\tau = \frac{1}{2} T_1$ LOCATED $\frac{1}{4}$ OF THE WAY ALONG T_2. (A SECOND GLIDE 3/4 OF THE WAY ALONG T_2 IS REPEATED FROM THE FIRST BY THE TRANSLATION $\frac{T_1+T_2}{2}$)



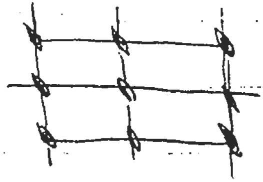
$\boxed{Cm}$

NOTE THE USE, FOR THE FIRST TIME, OF A "C" TO INDICATE A CENTERED LATTICE (THE m TELLS YOU ITS RECTANGULAR)

2mm + PRIMITIVE RECTANGULAR NET



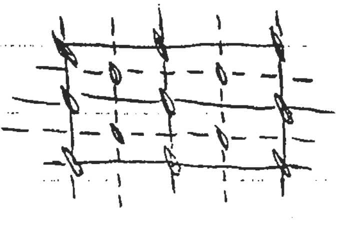
THIS INVOLVES ALL OF THE STEPS OF P2 PLUS ALL OF THE STEPS OF Pm FOR MIRROR PLANES ALONG BOTH EDGES OF THE CELL. THE WORK HAS ALL BEEN DONE AN THE RESULT IS OBVIOUSLY



$\boxed{P2mm}$

2mm + CENTERED RECTANGULAR NET

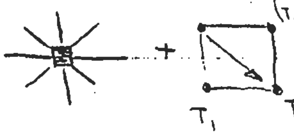
THIS IS ALL OF THE STEPS OF P2 PLUS ALL OF THE STEPS OF Cm FOR m'S IN 2 ORIENTATIONS. THE WORK HAS ALREADY BEEN DONE AND THE RESULT IS



$\boxed{C2mm}$

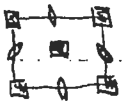
(. . . THIS IS THE NINTH SO FAR OBTAINED IF ANYBODY IS COUNTING)

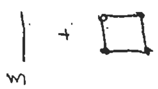
4mm:+ SQUARE NET

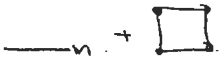


(T_2 is Symmetry Equivalent)

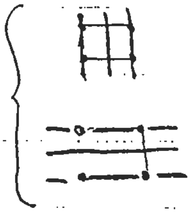
The 4-fold axis +  has Already been done in P4 ⇒



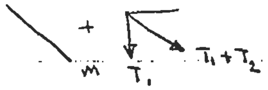




} has Already been done in pm ⇒

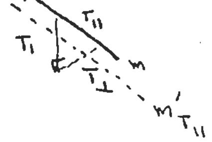


which Leaves



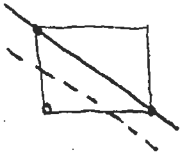
To be Considered (The other Diagonal mirror plane 90° Away is Symmetry-equivalent)

$(T_1+T_2)\cdot m = m'_{T_1+T_2} \equiv m$ ontop of the original m (T is ∥ to m) nothing new



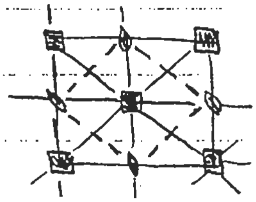
$T_1\cdot m = m'_{T_\parallel}$ @ $\frac{1}{2}T_\perp$ where $|T_\parallel| = |T_\perp| = T_1 \cos 45° = \frac{T_1}{\sqrt{2}}$

This is a new glide plane ⇒



Repeating planes by symmetry (e.g. Rotating the new glide at 90° intervals about the center of the cell)

Gives

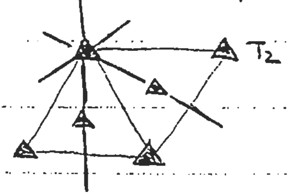


$\boxed{P4mm}$

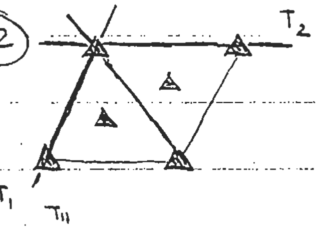
3m + Equilateral Net

Here we encounter a curious situation: The equilateral net has potentially a much higher symmetry than 3m and there are Two possible orientations for one and the same point group in the lattice

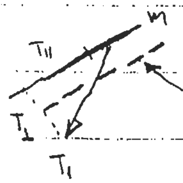
#1



#2



The 3-fold Axis makes T_1, T_2, and $-(\vec{T}_1+\vec{T}_2)$ Symmetry-equivalent, and All 3 mirror planes are equivalent so we need combine only 1 mirror with T_1 and reproduce the result by symmetry

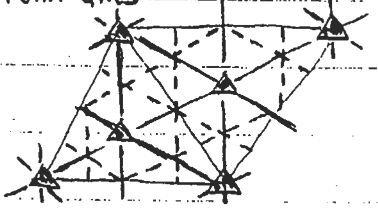


$T_1 \cdot m = m'_{T_\parallel}$ @ $\frac{1}{2}T_\perp$

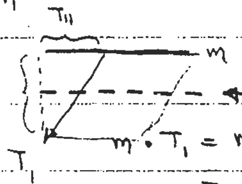
Glide component is $T_1 \cos 30° = T_1\frac{\sqrt{3}}{2}$

This is $\frac{1}{2}$ of the long diagonal of the cell.

Repetition of this glide by rotation with the two 3-fold axes in the interior of the cell and addition of 3m to every lattice point gives



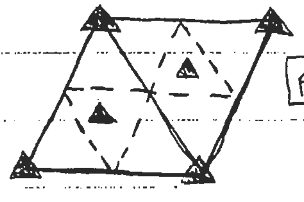
$\boxed{P3m1}$



$m\cdot T_1 = m'_{T_\parallel}$ @ $\frac{1}{2}T_\perp$

$T = T_\parallel = T_1 \cos 60° = \frac{1}{2}T_1$

Repetition of this glide by rotation with the two 3-fold axes in the interior of the cell gives:

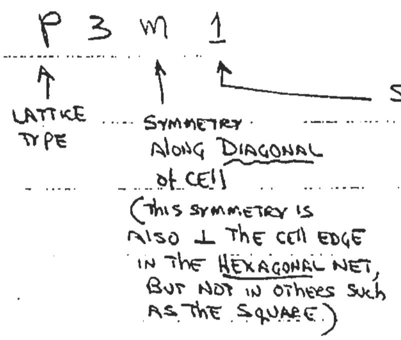


$\boxed{P31m}$

A thought before turning the page: Note that the plane groups above all contain (a) axes in the usual locations (b) mirror planes of the point group hung at lattice points.

Whenever a mirror is inclined to a translation in the net the effect is to interleave glides between all the mirror planes

In the above, the convention which we have used for establishing labels for the plane groups falls short — we can't simply call it p3m because for the first time we have obtained two distinct plane group from one and the same point group! Another convention is needed to distinguish between these results. The rule is to introduce another character into the point group part of the symbol to specify the symmetry which is along the diagonal of the cell (the long diagonal; the short one is symmetry-equivalent to the cell edge) as well as the symmetry along the cell edge: The order of symbols is



Happily, this situation occurs only for point group 3m !!

6mm + equilateral net We have already done all the work for this combination. Axes (6, 3 & 2-fold) occur in all of the locations of p6. We note that the mirror planes in 6mm are 30° apart, so the addition of 6mm to the lattice will place mirrors in the locations of both p31m and p3m1. The arrangement of mirrors and glides which thus results is simply that for p31m superposed upon p3m1. (We will unapologetically not try to sketch this one, and merely punt

$\boxed{P6mm}$

a drawing of the intricate arrangement of symmetry planes in this plane group is contained in the handout reproduced from the International Tables for X-ray Crystallography)

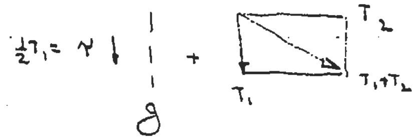
5.2 Replacement of Mirror Planes by Glide Planes

Thus far we have obtained 13 plane groups through direct addition of point groups to the 2-dimensional lattices. This might seem to exhaust all possibilities. But, in the process of these derivations, we were brought into headlong confrontation with the glide plane, a symmetry element which we had not encountered earlier as it exists only in translationally-periodic patterns and thus plays no role in the point groups.

In considering the space groups, however, one is dealing by definition with patterns that are translationally periodic, so glide planes may be present. One might ask, then, whether additional plane groups might be obtained by replacing mirror planes in the two-dimensional point groups by glides (which are, indeed, a generalization of a mirror plane in that m is a glide with $\tau = 0$) when two independent mirror planes are present in a point group, we might replace one or both by glides. The following replacements of m's by g's in a point group thus present themselves as possibilities which should be combined with the plane nets.

$$\left\{\begin{array}{l} m \rightarrow g \\ 2mm \rightarrow 2mg \text{ or } 2gg \\ 3m \rightarrow 3g \\ 6mm \rightarrow 6mg \text{ or } 6gg \end{array}\right.$$

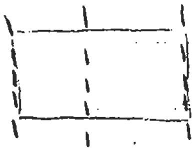
Replacing m by g : Addition of g to primitive rectangular net



$T_1 \cdot m_\tau = m'_{\tau+T_1}$ @ 0 Along T_2 $\equiv m_\tau$ Same glide on top of itself (Nothing new)

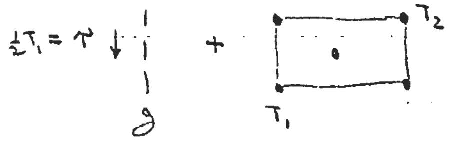
$T_2 \cdot m_\tau = m'_{\tau+0}$ @ $\frac{1}{2}$ Along T_2 A new glide halfway along the cell

$(\vec{T}_1+\vec{T}_2) \cdot m_\tau = m'_{\tau+T_1} \equiv m'_\tau$ @ $\frac{1}{2}$ Along T_2 Same new glide as above



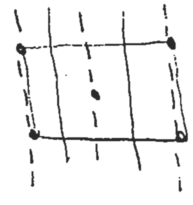
pg

Addition of g to centered rectangular net



Same combinations of operations as above in pg except for the new translation $\frac{1}{2}(\vec{T}_1 + \vec{T}_2)$ to the centered lattice point

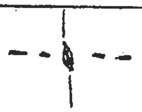
$\left(\frac{\vec{T}_1+\vec{T}_2}{2}\right) \cdot m_\tau = m'_{\tau+\frac{1}{2}T_1} \equiv m'_{T_1} \equiv m'$ @ $\frac{1}{4}T_2$ A new m $\frac{1}{4}$ Along T_2



This system of interleaved m's and g's is exactly that found for cm (Recall that there is no unique origin to a translation and no unique location for the lattice point)

Thus "cg" is identical to cm

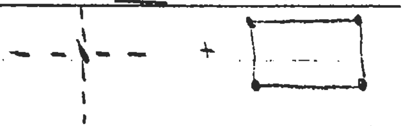
2mm with one m replaced by g



This combination is impossible. We have a theorem that states $\underbrace{m_1 \cdot A_\pi}_{\pi/2} = m_2$

so if one plane passing through the axis is a mirror, the second plane must also be a mirror.

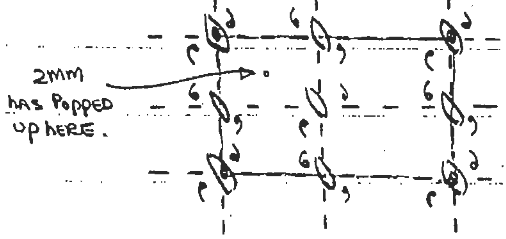
2mm with both m's replaced by g



The plane group c2mm (obtained by adding 2mm to a lattice point) was found to contain a 2-fold axis which had two glides passing through it. It thus would not be at all surprising to discover that if we began by adding 2gg a new location with symmetry 2mm would appear and the result turn out to be identical to c2mm. Let's show that this is the case.

2gg + Primitive rectangular net has all the combinations of p2 and pg (in two orientations)

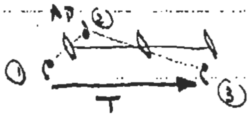
Therefore, on the basis of earlier combinations, the result is as shown to the left



We have not yet developed a combination theorem that tells us what the addition of a 2-fold axis to a glide – –⬮– – is equivalent to (we will do so in the next section) but if we draw in the pattern of p2 which is generated by the 2-fold axis, and then repeat these objects with the glides, we get the pattern shown to the left. This pattern is identical to that of c2mm referred to a different origin. Moreover, locations of symmetry 2mm are present at $\frac{1}{4}\frac{1}{4}$ $\frac{1}{4}\frac{3}{4}$ $\frac{3}{4}\frac{1}{4}$ $\frac{3}{4}\frac{3}{4}$ (anticipating the combination theorem we will derive) in addition, the lattice has been changed from a primitive rectangular net to a centered net

THE REASON FOR THIS MAY BE UNDERSTOOD BY PERMUTING A COMBINATION THEOREM WE HAVE PREVIOUSLY OBTAINED $T_{\perp} \cdot A_{\pi} = B_{\pi}$ @ 0 ALONG ⊥ BISECTOR

THEREFORE, TWO SUCCESSIVE ROTATIONS OF π ABOUT PARALLEL AXES IS EQUIVALENT TO A TRANSLATION EQUAL TO TWICE THE SEPARATION OF THE AXES $B_{\pi} \cdot A_{\pi} = T_{\perp}$



THUS THE PRESENCE OF A_{π} AT THE ORIGIN COMBINED WITH THE OPERATION B_{π} WHICH HAS APPEARED AT $\frac{1}{4}(\vec{T}_1+\vec{T}_2)$ REQUIRES THAT $\frac{1}{2}(\vec{T}_1+\vec{T}_2)$ BE A TRANSLATION

REPLACEMENT OF ONE m IN 4mm BY g

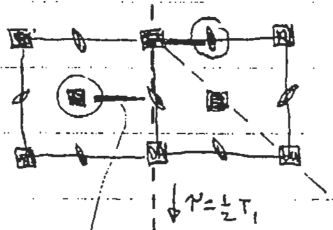
THIS COMBINATION IS AGAIN IMPOSSIBLE. THE THEOREM

$$\underbrace{m_1 \cdot A_{\frac{\pi}{2}} = m_2}_{\frac{1}{2}\frac{\pi}{2}}$$

REQUIRES THAT BOTH PLANES BE m IF ONE IS A MIRROR

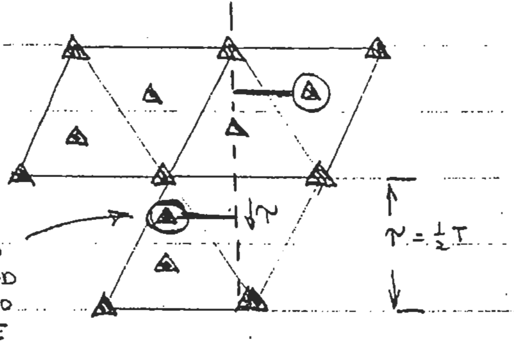
REPLACEMENT OF BOTH m'S IN 4mm BY g

THIS COMBINATION IS IMPOSSIBLE. A GLIDE CANNOT BE PLACED PARALLEL TO THE CELL EDGE OF P4 AS IT DOES NOT LEAVE THE AXES INVARIENT

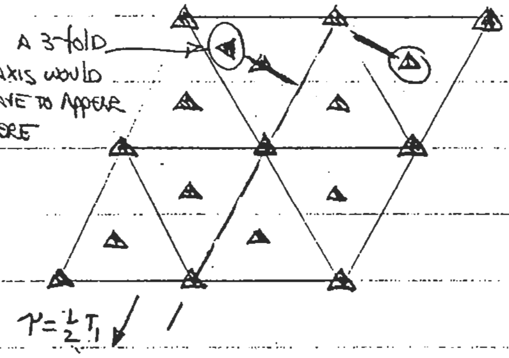


This would also have to be a 2-fold axis if a glide were present

ADDITION OF 3g1 31g OR 6gg TO THE EQUILATERAL NET (6gm IS IMPOSSIBLE)



A 3-fold axis would have to be here



A 3-fold axis would have to appear here

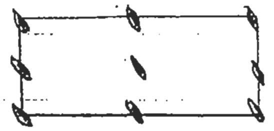
GLIDES ARE IMPOSSIBLE IN THESE ORIENTATIONS AS THEIR OPERATION DOES NOT LEAVE THE POSITIONS OF THE ROTATION AXES INVARIENT.

5.3 INTERLEAVING OF PLANES WITH AXES

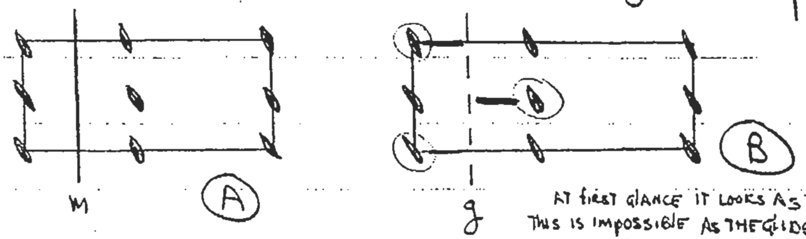
TO THIS POINT WE HAVE DERIVED 14 DISTINCT PLANE GROUPS AND THE WEARY READER HAS NO DOUBT SIGHED "SURELY WE HAVE NOW EXHAUSTED ALL THE POSSIBILITIES!". NOT QUITE YET. THE POTENTIAL COMBINATIONS WE HAVE THUS FAR EXAMINED HAVE ALL INVOLVED THE ADDITION OF EITHER A POINT GROUP (AXES; PLANES, OR PLANES PASSING THROUGH AXES) DIRECTLY TO A LATTICE POINT, OR A SIMILAR ADDITION IN WHICH ONE OR MORE OF THE MIRROR PLANES IN A POINT GROUP HAVE BEEN REPLACE BY A GLIDE. IN ALL OF THESE ADDITIONS ALL SYMMETRY ELEMENTS INTERSECTED AT A COMMON POINT WHICH, BY DEFINITION, THEY MUST DO IN A POINT GROUP AS A POINT IN SPACE MUST BE LEFT UNMOVED. THE PLANE GROUPS, HOWEVER, CONTAIN SYMMETRY ELEMENTS DISTRIBUTED THROUGHOUT SPACE; THERE IS NO LONGER ANY REASON, THEREFORE, WHY THE PLANES AND AXES WHICH WE ADD TO A LATTICE HAVE TO INTERSECT AT A COMMON POINT. AS THE FINAL STEP IN OUR DERIVATION WE SHOULD CONSIDER LOCATIONS WHERE, AFTER ADDING AXES TO A NET, WE CAN INTERLEAVE MIRROR PLANES OR GLIDE PLANES. THERE IS A CONSTRAINT IN DOING THIS: THE INTERLEAVED PLANES CANNOT CREATE ANY NEW TRANSLATIONS THROUGH THEIR OPERATION (FOR THIS WOULD CHANGE THE LATTICE NET WITH WHICH WE STARTED) NOR CAN IT CREATE ANY NEW ROTATION AXES (FOR THESE, IN TURN, WOULD CREATE NEW LATTICE POINTS THROUGH THEIR ACTION OR, ALTERNATELY, CREATE NEW TRANSLATIONS BY VIRTUE OF THE TRANSPOSED COMBINATION THEOREM $B_\alpha \cdot A_\alpha = T$ (A_α & B_α PARALLEL) WHICH WE ENCOUNTERED EARLIER AT THE TOP OF PG ⑪)

LET'S CONSIDER THE COMBINATIONS OF ROTATION AXES WITH THE PLANE NETS AND EXAMINE THEM FOR POTENTIAL LOCATIONS AT WHICH ONE MIGHT INTERLEAVE MIRRORS OR GLIDES (WE NEED NOT CONSIDER THE PARALLELOGRAM NET AS m OR g REQUIRES THAT ITS NET BE AT LEAST RECTANGULAR)

2 + PRIMITIVE RECTANGULAR NET

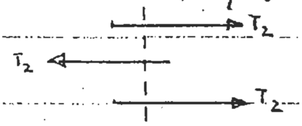


POTENTIAL LOCATIONS FOR INTERLEAVED m OR g



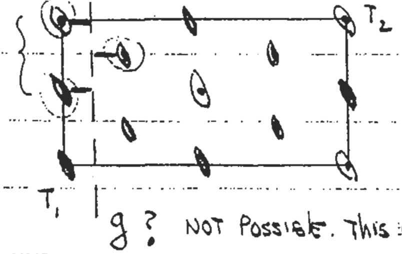
(WE WILL NOT REGARD THE INTERLEAVING OF m OR g IN AN ORIENTATION 90° FROM THAT SHOWN AS BEING DISTINCT AS THERE IS NOTHING SPECIAL ABOUT ONE EDGE OF THE RECTANGULAR CELL OR THE OTHER)

AT FIRST GLANCE IT LOOKS AS THOUGH THIS IS IMPOSSIBLE AS THE GLIDE WOULD SEEM TO CREATE A NEW LATTICE POINT AT THE CENTER OF THE CELL. REMEMBER, HOWEVER, THAT THERE IS NO UNIQUE PLACEMENT OF A LATTICE POINT, NO UNIQUE ORIGIN TO THE OPERATION OF TRANSLATION — ALL THAT IS SPECIFIED IS THE DIRECTION AND INTERVAL OF THE TRANSLATIONAL REPETITION. THUS THE ACTION OF THE GLIDE, ABOVE, IS TO REPEAT TRANSLATION T_2 THUSLY:



THIS CHANGES NEITHER THE MAGNITUDE OR DIRECTION OF T_2 AND, AS T_2 HAS NO UNIQUE ORIGIN, IS QUITE ACCEPTABLE

2 + CENTERED RECTANGULAR NET

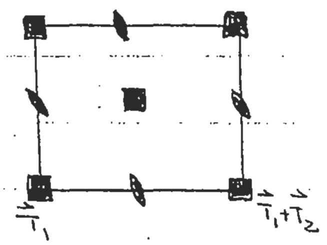


2Y = A TRANSLATION EQUAL TO $\frac{1}{2}T_1$ WHICH IS NOT PRESENT IN THIS LATTICE

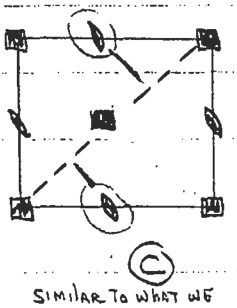
NOTHING POSSIBLE.

g? NOT POSSIBLE. THIS COMBINATION CREATES NO NEW 2-FOLD AXES, BUT $M_r^2 = \frac{1}{2}T_1$. THIS CREATES A NEW TRANSLATION $\frac{T_1}{2}$ IN THE LATTICE AND THUS CHANGES THE LATTICE. THIS COMBINATION REDUCES TO Ⓑ ABOVE.

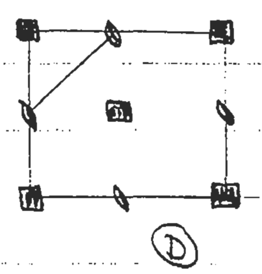
4 + Square net



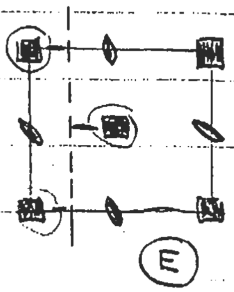
Potential locations for interleaved m or g



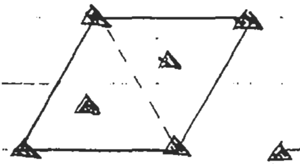
Similar to what we tried in placing 4gg at a lattice point, but now we are not adding a *pair* of glides 45° apart, but only *one*

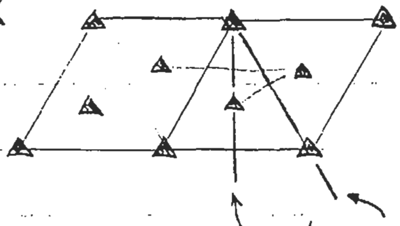


Not strictly an interleaved mirror plane, but a m can be accomodated in this position and in P4mm g occupied this location

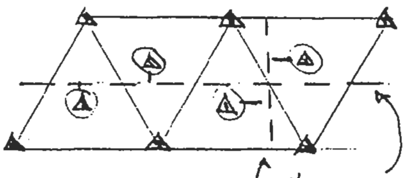


3 + Equilateral net





m's may be accomodated only in these positions (or symmetrically-equivalent locations) and we have already used them in P31m or P3m1 and in P6mm



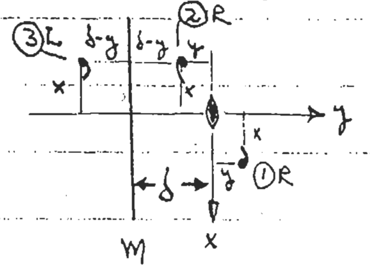
Glides may be accombdated in only these two locations, but they have already appeared there in P31m or P3m1 and in both positions for P6mm

Accordingly, there are *no new possibilities* for interleaving mirror planes or glides in combination with a 3-fold or 6-fold axis

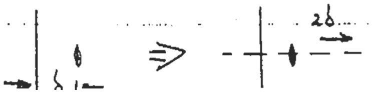
Thus, out of our considerations of possible positions for new plane groups involving m or g interleaved with axes have come 5 additional combinations of planes and axes — labeled Ⓐ through Ⓔ above — which must be examined as leading to potentially new plane groups.

Several of these (A, B & E) involve a combination of symmetry elements which we have not previously considered — namely the combination of a rotation operation with a plane which does *not* pass through the axis. In other cases (eg, C) we have a *glide* rather than a m passing through the rotation axes. These combinations will require an appropriate "combination theorem" to be established before proceding further. The necessary theorems may be viewed a generalizations of the theorem $m_1 \underbrace{\cdot A_\alpha}_{\alpha/2} = m_2$ which was developed in connection with derivation of the point groups.

Let us first consider the combination of A_π with a mirror plane which does not intersect the axis (but which is parallel to it) but is instead removed from the axis by a distance δ.



Let object ①, righthanded, say, be rotated to object ②R by the operation A_π. Let ②R be mapped to ③L by reflection in a plane removed from A_π by a distance δ. How is ①R related directly to ③L? They are of opposite handedness and must therefore be related by a mirror plane or glide. ① & ③ are symmetrically disposed at distance x on either side of the y axis, but are translated relative to one another in the y direction by an amount $\tau = y + y + (\delta - y) + (\delta - y) = 2\delta$. The new operation is thus

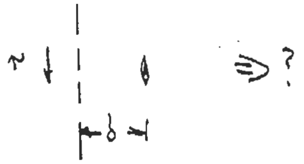


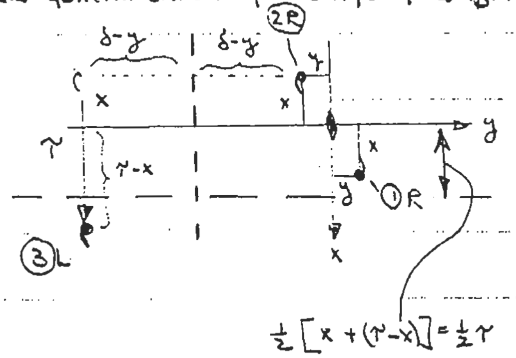
a glide with $\tau = 2\delta$ passing *through* the 2-fold axis and oriented 90° to the original mirror plane

Thus $$\boxed{\begin{array}{c} \overbrace{m \cdot A_{\pi} = m'}^{\frac{\pi}{2}}{}_{2\delta} \\ |\leftarrow \delta \rightarrow| \end{array}}$$

(As may be seen, any attempt to note the mutual orientation and position of the symmetry elements symbolically is rapidly becoming difficult)

Let's next consider a further generalization of this type of combination by making the original plane a glide



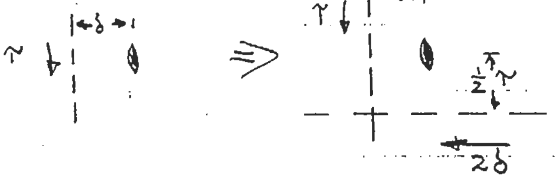


Objects ① & ③ remain, as above, separated in the y direction by an amount $\tau = y + y + (\delta - y) + (\delta -$

$= 2\delta$

The objects ① & ③ are again symmetrically disposed on either side of a line running in the y direction, but the line no longer passes through the 2-fold axis: it occurs at a value of x which is the average of the x coordinates of objects ① & ③, namely $\frac{1}{2}[x + (\tau - x)] = \frac{1}{2}$

Thus



Thus a glide with translation component τ combined with a 2-fold axis parallel to it, but separated by a distance δ, creates a new glide with translation component 2δ, at right angles to the initial glide and removed from the 2-fold axis by a distance $\frac{1}{2}\tau$

Any attempt to write this relationship symbolically should not be taken seriously, but let's try:

$$\boxed{\begin{array}{c} \overbrace{m_{\tau} \cdot A_{\pi} = m'}^{\frac{\pi}{2}}{}_{2\delta} \ \updownarrow \tfrac{1}{2}\tau \\ |\leftarrow \delta \rightarrow| \end{array}}$$

The more familiar theorem

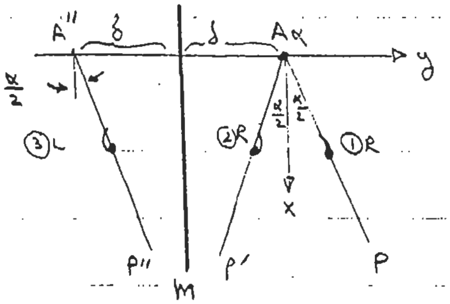
$$\underbrace{m \cdot A_{\pi} = m'}_{\frac{\pi}{2}}$$

may be seen to be a special case of this general result in which $\delta = 0$ and $\tau =$

(One further generalization of this theorem still remains for 3 dimensions where we will encounter screw axes. We could then replace A_{π} with a 2-fold screw operation.)

Combination of a plane with a general rotation operation

Let's now consider the case of a plane (m or g) combined with a general rotation operation A_{α}



Construct a line AP passing through the rotation axis A and making an angle $\frac{\alpha}{2}$ relative to the mirror.

The rotation operation A_{α} maps AP into AP'

The reflection operation maps AP' into A''P''.

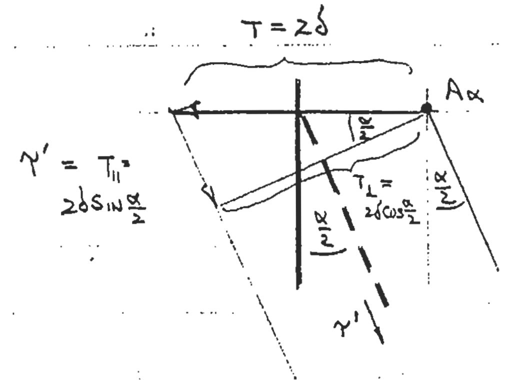
We can get directly from AP to A''P'' in the following two steps

(a) translate AP to A''P'' by an amount 2δ in the -y direction

(b) reflect things left-to-right across the line A''P'' to change handedness

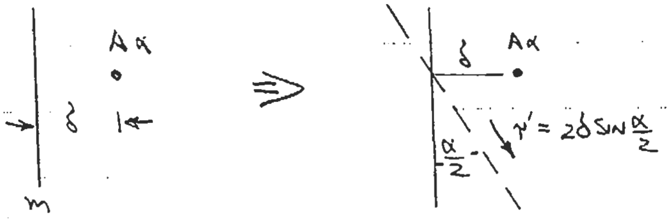
These two steps consist of reflection and translation in a direction inclined to the reflection plane. Let us combine these two steps into a single operation using a theorem which we had established earlier:

$$m \cdot T = m'_{T_{\parallel}} \ @ \ \tfrac{1}{2}T_{\perp}$$



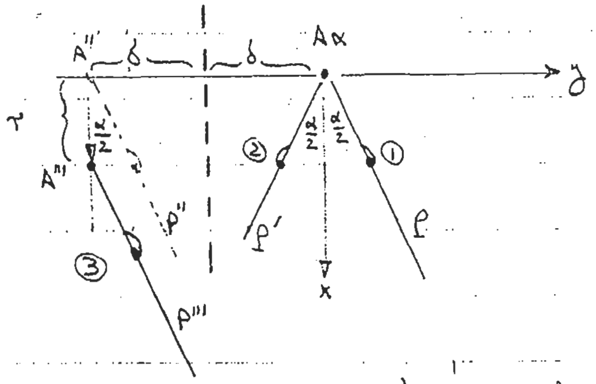
THE COMBINED MAPPING of $A\alpha$ followED BY REflECTION IN A PLANE PARALLEL TO THE AXIS BUT REMOVED BY A DISTANCE δ IS THUS A GLIDE WITH TRANSLATION COMPONENT $\tau' = 2\delta \sin\frac{\alpha}{2}$ INCLINED TO THE ORIGINAL MIRROR PLANE BY AN ANGLE $\frac{\alpha}{2}$. AND REMOVED from THE ROTATION AXIS BY A DISTANCE $\delta\cos\frac{\alpha}{2}$. THE NEW GLIDE INTERSECTS THE INITIAL MIRROR PLANE AT THE POINT WHERE A PERPENDICAL BETWEEN THE AXIS AND m INTERSECTS THE MIRROR

Thus



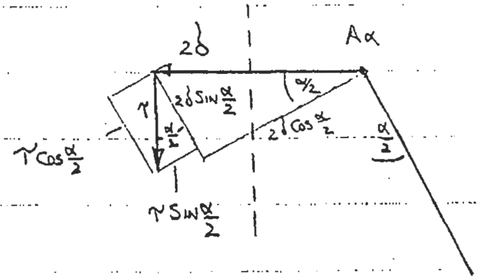
(CONVERSELY, COMBINING m with g AT ANGLE $\frac{\alpha}{2}$ CREATES A ROTATIONAL OPERATION $A\alpha$ AT A POINT REMOVED from the LINE of INTERSECTION of THE TWO PLANES)

COMBINATION of A GLIDE PLANE with A PARALLEL ROTATION OPERATION AT A DISTANCE



ROTATION OPERATION $A\alpha$ MAPS AP TO AP′
THE GLIDE OPERATION REFLECTS AP′ TO A″P″
AND THEN TRANSLATES TO A‴P‴

WE CAN MAP AP INTO A‴P‴ DIRECTLY BY TRANSLATING AP BY 2δ ALONG -y AND τ ALONG x followED BY REFLECTION ACROSS A‴P‴ TO CHANGE HANDEDNESS



AGAIN $m \cdot T = m'_{T_{\parallel}} @ \frac{1}{2} T_{\perp}$

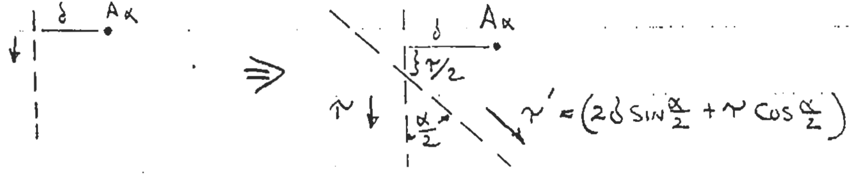
here $T_{\perp} = 2\delta\cos\frac{\alpha}{2} + \tau\sin\frac{\alpha}{2}$

$T_{\parallel} = 2\delta\sin\frac{\alpha}{2} + \tau\cos\frac{\alpha}{2}$

THE COMBINED EFFECT of ROTATION THROUGH AN ANGLE α followED BY GLIDE IN A PLANE REMOVED from THE AXIS BY A DISTANCE δ IS THUS GLIDE IN A NEW PLANE LOCATED $\frac{\alpha}{2}$ AWAY from THE FIRST, HAVING TRANSLATION COMPONENT $\tau' = \left(2\delta\sin\frac{\alpha}{2} + \tau\cos\frac{\alpha}{2}\right)$ AND REMOVED from the ROTATION AXIS BY A DISTANCE $\delta' = \left(\delta\sin\frac{\alpha}{2} + \frac{\tau}{2}\cos\frac{\alpha}{2}\right)$

WHERE DOES THIS NEW GLIDE INTERSECT THE FIRST? $\frac{1}{2}$ of THE PERPENDICULAR COMPONENT of THE TRANSLATION COMPONENT $\overrightarrow{2\delta}$ WOULD PLACE THE GLIDE AT THE INTERSECTION of THE ORIGINAL GLIDE AND THE PERPENDICULAR TO $A\alpha$. ONE-half of THE SECOND PART of THE TRANSLATION, $\vec{\tau}$, SLIDES THE POINT of INTERSECTION $\frac{1}{2}\tau$ ALONG THE ORIGINAL GLIDE.

Thus



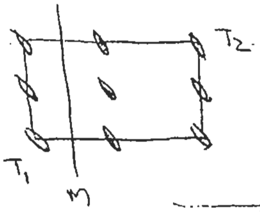
This most general theorem for two dimensions will also need a further generalization for three dimensions; replacement of A_α, a pure rotation, by a screw operation.

Before proceding to complete our derivation it is perhaps worth repeating what we are doing, in the language of group theory. In deriving the point groups, for example, we took a <u>subgroup</u> (a combination of rotation axes, for example) and added to this group of operations an additional operation (such as a horizontal mirror plane, for example) called an <u>extender</u>; for the new collection of operations to qualify as a group, the combination of any two elements also has to be a member of the group. If a particular combination of elements provides an effective net operation which is not an element in the extended set, we add the new operation to the group. We check this by means of constructing the "Group Multiplication Table"

We are performing the same operation here, the only difference being that a plane group is an <u>infinite group</u>, rather than being a <u>finite</u> group with a small number of elements as is the case with a point group. To a subgroup (eg, a plane group such as P2) we add a new extender operation such as an interleaved or intersecting reflection or glide. We then combine this new operation with the operations of the subgroup (translations terminating within the cell; existing rotation operations in the subgroup) constructing, in effect, the group multiplication table. The "combination theorems" we have established as general results tell us the result of the "product" of a given pair of operations. If the result is already a member of the group (eg, a mirror operation which falls on top of a mirror plane which is already in the pattern) we discard it — it is nothing new; an operation which is already a member of the group. If the result is a new operation which is <u>not</u> already in the group we must add it to the collection of elements which constitute the group.

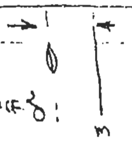
Returning to the five remaining possibilities for combining planes and axes (which we have identified on pg 12 & 13:

Ⓐ

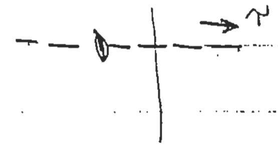


[We will omit the steps which we have seen do not lead to new symmetry elements eg, $m \cdot T_1 = m'_{T_1} \equiv m'$ right on top of the original m; thus nothing new]

$T_2 \circ m = m' @ \frac{1}{2}T_2$

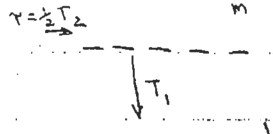


$\Rightarrow$



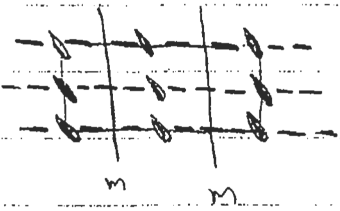
$\rightarrow \tau = 2\delta = 2\cdot\frac{1}{4}T_2 = \frac{1}{2}T_2$

Theorem at bottom of pg 13 for combining A_π with a m separated by distance δ:



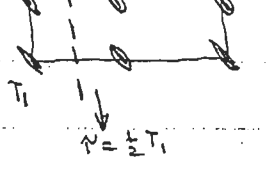
$= T_1 \circ m_{\frac{1}{2}T_2} = m'_{\frac{1}{2}T_2} @ \frac{1}{2}T_1$

Final result



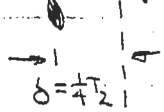
$\boxed{p2mg}$

Ⓑ

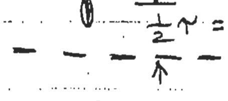


$T_2 \cdot m_{\frac{1}{2}T_1} = m'_{\frac{1}{2}T_1} @ \frac{1}{2}T_2$ from our initial glide — ie, at $\frac{3}{4}T_2$.

Theorem at middle of pg 14 provides



$\Rightarrow$

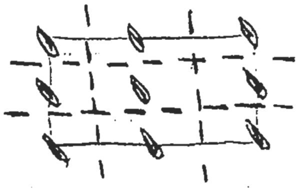


$\rightarrow \tau' = 2\delta = 2\cdot\frac{1}{4}T_2 = \frac{1}{2}T_2$

THE NEW GLIDE $\frac{1}{4}$ ALONG T_1 WITH $\tau = \frac{1}{2}T_2$ will BE REPEATED AGAIN AT $\frac{3}{4}T_1$

$\left(T_1 \cdot m_{\frac{1}{2}T_2} = m'_{\frac{1}{2}T_2} \text{ @ } \frac{1}{2}T_1 \text{ from ORIGINAL GLIDE AT } \frac{1}{4}T_1 \right)$

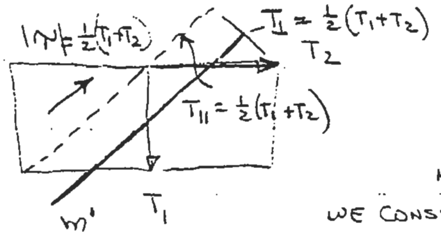
final RESULT



$\boxed{p2gg}$

TURNING NEXT TO THE THREE POSSIBILITIES Ⓒ Ⓓ & Ⓔ ON THE TOP of Pg 13 for THE SQUARE NET

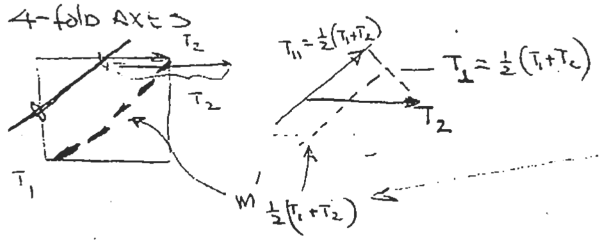
Ⓒ



$$T_2 \cdot m_{\frac{1}{2}(T_1+T_2)} = m'_{\frac{1}{2}(T_1+T_2)+\frac{1}{2}(T_1+T_2)} \equiv m'_0 \text{ AT } \frac{1}{2}\cdot\frac{1}{2}(T_1+T$$

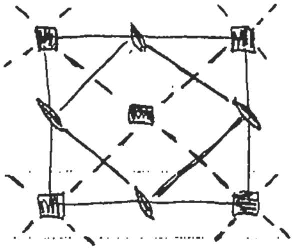
NOTE THAT THIS NEW MIRROR PLANE IS THE ONE which WE CONSIDERED. ADDING INITIALLY IN POSSIBILITY Ⓓ

Ⓓ IN light of THE ABOVE IT WOULD BE NOT AT ALL SURPRISING TO find THAT if WE START BY ADDING THE MIRROR PLANE THROUGH THE 2-fold AXIS, WE GET A GLIDE PASSING THROUGH THE 4-fold AXES

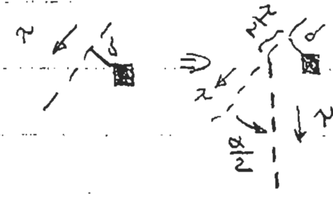


$$T_2 \cdot m = m'_{\frac{1}{2}(T_1+T_2)} \text{ @ } \frac{1}{2}\cdot\frac{1}{2}(T_1+T$$

Both Ⓒ & Ⓓ THUS LEAD TO THE SAME RESULT. THE GLIDE & MIRROR PLANE, WHEN REPEATED BY THE 4-fold AXES GIVES for Both Ⓒ & (



WE STILL HAVE NOT CONSIDERED THE Effect of COMBINING A 4-fold AXIS with A GLIDE PASSING THROUGH IT. USING THE THEOREM AT THE BOTTOM of Pg 15



$$\tau' = 2\delta \sin\frac{\alpha}{2} + \tau \cos\frac{\alpha}{2}$$

IN THE PRESENT CASE $\delta = 0$ SO THE NEW GLIDE has

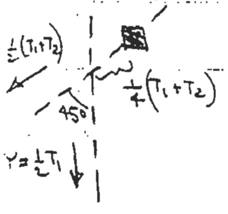
$$\tau' = \underset{0}{2\cdot 0 \sin\frac{90^\circ}{2}} + \tau \cos\frac{90^\circ}{2}$$

$$\tau' = \tau \cos 45^\circ = \frac{\tau}{\sqrt{2}}$$

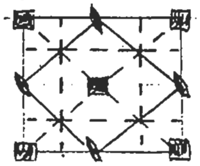
BUT THE ORIGINAL τ IN THE first GLIDE PLANE HAD MAGNITUDE $\frac{1}{2}|\vec{T}_1 + \vec{T}_2| = \frac{1}{2}|T_1|\sqrt{2} = \tau$

SO $\tau' = \frac{1}{2}|T_1|\sqrt{2}/\sqrt{2} = \frac{1}{2}T_1$

THE RESULT IS ~~NOT~~ ANOTHER GLIDE, THIS ONE PARALLEL TO THE CELL EDGE. AND GOLLY, GUESS WHAT? THIS IS PRECISELY THE THIRD AND final POTENTIAL LOCATION for A GLIDE, IDENTIFIED ABOVE AS Ⓔ. If WE STARTED WITH THIS ADDITION of A GLIDE, THE REVERSE of OUR PRESENT COMBINATION THEOREM WOULD HAVE FED BACK THE GLIDE ALONG THE DIAGONAL of [illegible]



Ⓒ, Ⓓ & Ⓔ All THUS LEAD TO THE SAME RESULT



$\boxed{p4gm}$