## Section 2.12 Two-dimensional Space Groups

The reader will probably agree that the derivation of the primitive lattice types and space groups in three-dimensional space is complicated. Therefore, as a change of pace we present here the corresponding results in two-dimensional space. The primary advantage of working in the plane over working in three-space is the ease of visualization of lattice types. Furthermore the results are much simpler to state: There are five lattice types and only 17 isomorphism classes of two-dimensional space groups.

The definitions of two-dimensional lattices, lattice groups, basic vectors, crystallographic point groups, holohedries, space groups, etc. are mere paraphrases of definitions of the corresponding three-dimensional objects. We will not bore the reader with these details but will merely comment on the essential steps in the argument leading to the classification of the two-dimensional space groups. (Note: Two-dimensional lattices are often called nets.)

At the end of Section 2.5 the possible point groups in the plane were listed: the cyclic groups  $C_n$  and the dihedral groups  $D_n$ ,  $n=1,2,\cdots$ . We will determine which of these are crystallographic point groups.

It follows immediately from the proof of theorem 2.7 that for any two-dimensional lattice group H there exist linearly independent vectors  $b_1, b_2$  such that every  $a \in H$  can be written uniquely in the form  $a = \gamma_1 b_1 + \gamma_2 b_2$ ,  $\gamma_1 \gamma_2$  integers.

The  $b_1$  are <u>basic vectors</u> for H and the parallelogram Q that they generate is a <u>primitive cell</u>. The area A(P) of the cell P generated by two arbitrary linearly independent vectors  $b_1, b_2 \in H$  is an integer multiple of A(Q). Furthermore, A(P) = A(Q) if and only if  $b_1, b_2$ 

are basic vectors for H. Given any  $Q \in H$  there always exist basic vectors  $b_1, b_2$  for H such that  $b_1$  lies on the line segment through  $\theta$  and q. In fact we can require that  $b_1$  is the non-zero lattice vector on Q which is closest to q. (We are considering the lattice group H as an additive group whose elements are vectors in  $R_2$ . The zero vector q is the identity element of H.)

Let K be a crystallographic point group in the plane, i.e., K is a symmetry group of a two-dimensional lattice (or net) L which fixes a given point X \( \) L. For convenience we choose X \( \) \( \) An argument almost identical with the proof of theorem 2.9 shows that the crystallographic restriction is still in effect. That is, K can contain non-trivial rotations only if their orders are 2, 3, 4 or 6. This proves that no point group which contains rotations of order 5 or greater than 6 can be crystallographic point groups. Thus there are only ten possible crystallographic point groups:

(12.1) C1,C2,C3,C4,C6,D1,D2,D3,D4,D6.

We shall show that in fact each of these ten groups is a point symmetry group of some two-dimensional lattice.

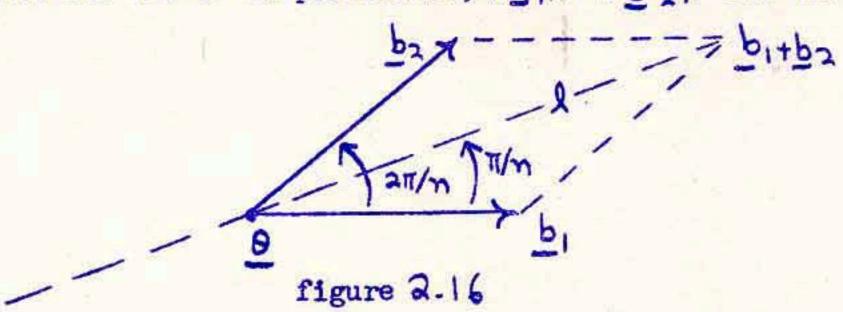
Proceeding as in the three-dimensional case we next try to determine the holohedries of two-dimensional lattices. Let  $\bot$  be a net based at  $\times = \Theta$  and let  $\top$  be its holohedry (maximal point symmetry group) at  $\times$ . Now the rotation  $\subseteq_{\mathbb{T}}$  of 180° about  $\Theta$  is always an element of  $\top$ . Indeed, if  $b_1, b_2$  are basic vectors for  $\bot$  then

(12.2)  $C_{\pi}b_1 = -b_1$ ,  $C_{\pi}b_2 = -b_2$ .

It follows that  $C_{\pi}$  maps L into itself, so  $C_{\pi} \in F$ . Therefore,  $C_1$ ,  $C_3$ ,  $D_1$  and  $D_3$  cannot be holohedries since they do not contain  $C_{\pi}$ .

(This result is the two-dimensional analogy of theorem 2.10.)

Similarly, in analogy with theorem 2.11 we can show that if F contains  $C_n$ , n=3,4,6 then F contains  $D_n$ . To prove this we let C be the rotation through the angle  $2\pi/n$ , n=3,4 or 6, and  $b_1$  be a vector of minimum nonzero length in L. An argument identical with that immediately following figure 2-9 shows that  $b_1$  and  $b_2=Cb_1$  are basic vectors for L. In particular,  $\|b_1\|=\|b_2\|$  and the angle between



b) and b2 is  $2\pi/n$ . To prove that F contains  $D_n$  it is enough to show that F contains the reflection R in the line I which bisects the angle between b1 and b2. (The lattice point b1+b2 lies on I.) Indeed, C and R generate  $D_n$ . Now it is obvious that  $Rb_1=b_2$ ,  $Rb_2=b_1$ . Therefore, R maps L into itself and  $R\in F$ . This result shows that  $C_3$ ,  $C_4$  and  $C_6$  cannot be holohedries.

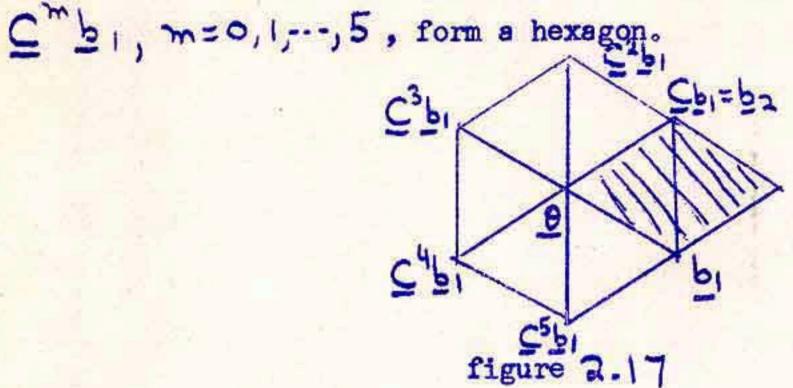
We conclude that there are at most four holohedries:

To show that each of these groups is a holohedry it is necessary to construct a lattice which admits the group as its holohedry.

Just as in the three-dimensional case, we take up the possible holohedries one at a time and determine the lattice types (or <u>net types</u>) which correspond to them.

The hexagonal holohedry D6: Suppose L is a net based at 8 which

admits  $D_6$  as its holohedry, and let  $C \in D_6$  be the rotation through  $\sqrt[4]{3}$  about O. As remarked above, we can choose  $b_1$ ,  $Cb_1$  as basic vectors for L where  $b_1 \in L$  is of minimal nonzero length. The net L is now completely determined! In particular we see that the lattice points



It is now clear that may lattice  $\bot$  constructed from basic vectors  $\underline{b}_1, \subseteq \underline{b}_1$  admits  $D_6$  as a crystallographic point group. In particular three of the two-fold axes  $l_1, l_2, l_3$  of  $D_6$  pass through  $\underline{\theta}$  and  $\underline{b}_1, \subseteq \underline{b}_1, \subseteq 2\underline{b}_1$ , respectively. The remaining three two-fold axes bisect the angles between adjacent  $l_1$ . The primitive cell generated by  $\underline{b}_1, \subseteq \underline{b}_1$  is denoted  $N_b$ . Type  $N_b$  nets must necessarily admit  $D_6$  as a holohedry since  $D_6$  is not a proper subgroup of any of the possible holohedries in the list (12.3). Clearly, type  $N_b$  nets can be uniquely determined by the single parameter  $\|\underline{b}_1\|_6$ . We have shown that the hexagonal crystal system contains the single net type  $N_b$ .

The tetragonal holohedry  $D_4$ : Suppose  $\bot$  is a net based at B which admits  $D_4$  as its holohedry and let  $C \in D_4$  be the rotation through  $\mathbb{T}/2$  about B. Then we can choose  $B_1, C_2$  as basic vectors for L where  $B_1$  is a net vector of minimal nonzero length. Clearly the primitive cell  $N_4$  generated by these basic vectors is a square. Thus L is completely

determined. The reader can easily check that any type  $N_Q$  net admits  $D_Q$  as a symmetry group. Furthermore,  $D_Q$  must be the holohedry of a type  $N_Q$  net since  $D_Q$  is not a proper subgroup of any of the possible holohedries (12.3). Type  $N_Q$  nets can be described by the single parameter  $\|b_Q\|$ . We have shown that the tetragonal crystal system contains the single net type  $N_Q$ .

The orthorhombic holohedry  $D_2$ : Suppose  $\bot$  is a net with holohedry  $D_2$  and let  $C \in D_2$  be the rotation through T about D. Let L be one of the two-fold reflection exes and  $R \in D_2$  the reflection about L. Necessarily, L passes through at least one lattice point. Indeed if L then L L is a lattice point such that L L L L therefore, we can choose basic vectors L L for L such that L lies on L . Write

(12.4)

where U is parallel to  $b_1$  and V  $Lb_1$ . Clearly  $Rb_2 = U - V$ 

SO

(12.5)

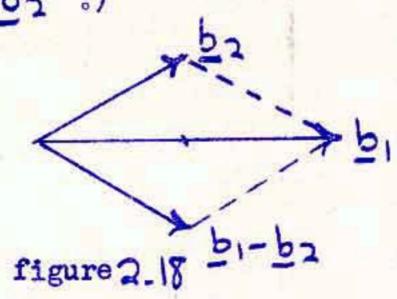
Rb2+b2 = 2UEL.

It follows that  $2u = \gamma_1b_1$  where  $\gamma_1$  is an integer, or  $u = \frac{\gamma_1}{2}b_1$ . We can subtract integral multiples of  $b_1$  from  $b_2$  without changing the area of the primitive cell. Therefore, we can assume that either  $\gamma_1 = 0$  or  $\gamma_1 = 1$ . It now follows from (12.5) that there are two possibilities: Either 1)  $k = b_1 = b_2$  in which case  $k = b_1 + k_2 = b_1 + k_2 = b_1 + k_2 = b_1 + k_2 = b_2 = b_1 + k_2 = b_2 = b_1 + k_2 = b_2 = b_$ 

We take case 1) first. The basic vectors generate a rectangle  $N_{\gamma}$ . Since C and R generate D<sub>2</sub> it is clear that a type  $N_{\gamma}$  net admits D<sub>2</sub>

as a symmetry group. In order that  $D_2$  be the holohedry it is necessary and sufficient that  $N_{\gamma}$  not be a square. (Otherwise the holohedry would be  $D_{\gamma}$ .) A type  $N_{\gamma}$  net is determined by two parameters:  $\|b_1\|$  and  $\|b_2\|$ .

In case 2) the basic vectors  $b_1 - b_2$  and  $b_2$  generate a rhombus  $N_V$ . (Note:  $N_V$  is a primitive cell since it has the same area as the primitive cell generated by  $b_1$  and  $b_2$ .)



It is now clear that a type  $N_{\Upsilon}$  net admits  $D_2$  as a symmetry group. Furthermore  $D_2$  is the holohedry as long as the angle between  $b_1-b_2$  and  $b_2$  is not  $\pi/2$  or  $\pi/3$ . A type  $N_{\Upsilon}$  net is determined by two parameters:  $\|b_2\|$  and the angle between  $b_1-b_2$  and  $b_2$ .

We have shown that the orthorhombic crystal system contains two net types,  $N_{\tau}$  and  $N_{\mathcal{V}}$ .

The monoclinic holohedry  $C_2$ : Every net admits  $C_2$  as a symmetry group. Thus,  $C_2$  is a holohedry for those nets which do not belong to the other lattice types listed above. Let L be such a net. We choose basic vectors  $b_1, b_2$  for L of minimal nonzero length. Let  $N_a$  be the corresponding primitive cell. By comparing with the lattice types listed above we see that a type  $N_a$  net admits  $C_2$  as its holohedry if and only if  $\|b_1\|$   $\#\|b_2\|$  and  $\|b_1\|$  is not perpendicular to either  $\|b_2\|$  or  $\|2b_2-b_1\|$ . A type  $N_a$  net is determined by three parameters:  $\|\|b_1\|$ ,  $\|\|b_2\|$  and the angle between  $\|b_1\|$  and  $\|b_2\|$ .

## figure 2.19

	crystal system (holohedry)		crystal classes	net types
1.	monoclinic	Ca	C2, C1	Na
2.	orthorhombic	D <sub>2</sub>	$D_2, D_1$	Nr, Nr
3.	tetragonal	04	D4, C4	Nq
4.	hexagona1	D <sub>6</sub>	D6,C6,D3,C3	Nh

The procedure for deducing two-dimensional space groups G from the above table is almost identical (but simpler) than the procedure for three-dimensional space groups. In particular the material following equation (10.3) is applicable if we read O(2), E(2), T(2) for O(3), E(3), T(3).

We now know that the ten groups (12.1) are indeed crystallographic point groups, since they are all subgroups of holohedries. Each of these groups defines a crystal class. Moreover, the crystal class K is assigned to the crystal system with the smallest holohedry F containing K. This assignment of crystal classes to crystal systems is indicated in figure 2-19.

Any two-dimensional symmorphic space group G is obtained by choosing a net type H, i.e., a two-dimensional lattice group corresponding to a certain net type, and a crystal class K leaving H invariant. G is the semi-direct product of H and K. In the monoclinic system there are two crystal classes and one net type, which yield two symmorphic groups. The orthorhombic system has two crystal classes and two net types, yielding

four symmorphic groups. Continuing in this way we get twelve symmorphic groups. There is actually one more, due to the fact that the crystal class  $D_3$  can act on the hexagonal lattice in two distinct ways. Either the three reflection axes of  $D_3$  lie along  $b_1$ ,  $Cb_1$  and  $C^2b_1$  in figure 2.17 or they bisect the angles between adjacent vectors  $C^3b_1$ . Thus, there are a total of thirteen two-dimensional symmorphic groups.

We now proceed to the deduction of the non-symmorphic groups. Let G be a space group and let n = 1, 2, 3, 4 or G be the order of the rotation axis of its crystal class K. If G is the rotation of angle  $2\pi/n$  in K, there must exist a unique element  $\{a_1, G\}$  in G such that

where  $b_1, b_2$  are basic vectors for the net type of G . It follows from the identity

(12.6) 
$$T_{\underline{\alpha}} \{ \underline{\alpha}_{1}, \underline{C}_{3} \} T_{\underline{\alpha}} = \{ \underline{\alpha}_{1} + \underline{\alpha} - \underline{C}_{\underline{\alpha}}, \underline{C}_{3} = \{ \underline{\theta}_{1}, \underline{C}_{3} \}$$
where

that G is conjugate to a space group  $G = T_{\alpha} G T_{\alpha}$ . Thus, in the conjugacy class to which G belongs there is a space group G containing the elements  $\{0, C^m\}$ , m=1,2,...,m-1. For simplicity we will always choose the space group G in each conjugacy class. It is an immediate consequence of this result that all space groups belonging to the crystal classes  $C_{1,1}C_{2,1}C_{3,1}C_{4}$  and  $C_{4}$  are symmorphic. Only space groups G belonging to the crystal classes  $D_{m,1}m=1,2,3,4$  or  $G_{m,2}m=1,2,3,4$  or  $G_{m,3}m=1,2,3,4$  or  $G_{m,4}m=1,2,3,4$  or  $G_{m,4}$ 

The exact definitions of b, b, for the various net types have been described above.

Since

(12.9) 
$$\{a_2, R_3^2 = \{R_{21} + a_2, E_3 \in H\}$$

it follows that there exist integers NIN2 so that

We will compute 22 -

First consider the crystal class  $D_1$  and net type  $N_{\Upsilon}$ . We can assume  $Rb_1=b_1$  and  $Rb_2=-b_2$ . (Recall  $b_1\bot b_2$  for  $N_{\Upsilon}$ .) Then  $Ra_2+a_2=2\alpha,b_1=n,b_1+n_2b_2$ ,

so d, = 0 or 1/2 . Furthermore, the identity

(12.11)  $T_{a} = \{ \alpha_{1}b_{1} + \alpha_{2}b_{2}, R \} T_{a}^{-1} = \{ \alpha_{1} - R\alpha + \alpha_{1}, R \} = \{ \alpha_{1}b_{1}, R \}$ where  $\alpha = -\frac{1}{2}\alpha_{2}b_{2}$  shows that we can assume  $\alpha_{1} = 0$ , i.e., G is conjugate to a space group G with the same net group H and containing  $\{ \alpha_{1}b_{1}, R \}$ . Therefore we have exactly two possible space groups of class D, and type  $N_{Y}$ :

(12.12)  $C_s^{T}: \{0, R\}$   $C_s^{T}: \{b\}, R\}$ 

Note that each of these space groups are generated by the lattice group  $\mathbb{N}_{\mathbf{r}}$  of type  $\mathbb{N}_{\mathbf{r}}$  and the element  $\mathbb{N}_{\mathbf{r}}$  is symmorphic. However, the non-symmorphic group  $\mathbb{N}_{\mathbf{r}}$  is new.

Leave the crystal class fixed, but change the net type to  $N_T$ . We can now assume that  $Rb_1=b_1$ ,  $Rb_2=b_1-b_2$ . Thus,

(12.13) Raz+Qz = (2d1+d2)b1 EH.

Furthermore, applying a conjugacy transformation of the form (12.11) we find  $Ta \{ \alpha_{1}b_{1} + \alpha_{2}b_{2}, R \} Ta^{-1} = \{ \alpha_{2} - R\alpha + \alpha, R \}$ 

if  $Q = \alpha_1 b_1$ . It follows from (12.13) applied to  $Q_1$  that  $Q_2 \in H$ . Thus, G is conjugate to a space group containing  $\{Q, R\}$  and the only space group of class  $D_1$  and type  $N_Y$  is symmorphic.

Next consider a space group G of class  $D_2$  and type  $N_v$ . Let G be the rotation through  $\pi$  and  $G \in D_2$  a reflection. We can assume

Eurthermore, as remarked above we can assume  $C' = \{0, C\} \in G$ . Choose  $R' = \{a_1, R\} \in G$  with  $a_1 = \alpha_1 b_1 + \alpha_2 b_2$ ,  $0 \le \alpha_1, \alpha_2 < 1$ . The relation  $R^2 = E$  implies  $Ra_1 + a_1 \in H$  or  $a_1 = \alpha_1 b_1 \in H$ . Similarly, the relation  $(CR)^2 = E$  or  $(\{0, C\} \{a_1, R\})^2 \in H$ implies  $CRa_1 + a_1 \in H$  or  $a_1 + a_2 \in H$ . There are four possibilities:

Note that G is uniquely determined by G' and R'. Case 1) yields the symmorphic group  $G_{2V}$ . Cases 2) and 3) obviously yield isomorphic groups (since there is another reflection in  $D_2$  fixing  $b_2$ ). We select case 2) and obtain the non-symmorphic group

Case 4) yields the non-symmorphic group

If G is of class D2 and type Ny we can assume

The relation  $(CR)^2$ = Eimplies  $CRa_1 + a_2 = -(a_1 + a_2)b_1 + a_2b_2 \in H$ . Thus,  $a_2 = a_1 = 0$  and G is symmorphic.

Next, suppose G is of class D3 and (necessarily) type Nh . Let  $C \in O_3$  be the rotation through  $2\pi/3$ . Then we can assume  $C = \{0, C\} \in G$ and Cb1=b2-b1, Cb2=-b1. We can choose a reflection R&D3 such that it acts on  $N_h$  in one of two possible ways: Either 1)  $Rb_1 = b_1$ , Rb2=b1-b2 or 2) Rb1=b2, Rb2=b1. (This embiguity is due to the fact that D3 can act as a crystallographic point group in a type  $N_{h}$ -net in two distinct ways.) Suppose  $R' = \{a_1, R\}$  (G with  $a_1 = \{a_1, R\}$ )  $\alpha_1 b_1 + d_2 b_2$ ,  $0 \le \alpha_1, \alpha_2 \le 1$ , and consider case 1). The relation (R'C') + arising from (RC)2=E, implies RCa1+a1= (201-d2)b1+ (d2-2d1)b2 eH. Furthermore, R12 eH implies Raita1= (2d1+d) b1 eH. These two relations imply  $2\omega_1=0,1$  and  $\omega_2=0$ . Finally  $(RC^2)^2=E$ implies RC a,+a, = (d,+2d2) b26H, so d,=d2 = 0. Thus G is symmorphic. Case 2) can be treated in the same way and yields only a single symmorphic group.

Now consider a space group of class Dy and type No. If C & Dy is the rotation through  $\pi/2$  and  $R \in D_4$  is a reflection, we can assume

Cb1=b2, Cb2=-b1, Rb1=b1, Rb2=-b2. Furthermore, we can assume 10,5366 and 5a1,R366 with a = dib1+d2b2)  $0 \le \alpha_1, \alpha_2 < 1$ . The relation  $\mathbb{R}^2 = \mathbb{E}$  yields  $\mathbb{R}_a, +\alpha_1 = 2\alpha_1 b_1 \in \mathbb{H}$ , so 22,=0,1. Similarly, the relation (RC)2=E yields RCa1+a1 = (d,-d,)(b,-b) eH. There are two possibilities:

CT: 30, R3 d1=d2=0

 $C_{4V}^{I}: \{\{\{b_1+b_2\}\}, R\}$   $(a_1=\alpha_2=1)_2$ The group  $C_{4V}^{I}$  is symmorphic, but  $C_{4V}^{II}$  is not. (It is easy to verify that, in fact, CHV is a uniquely determined space group.)

The last space group G to consider is one of class DG and type Nh .

Let  $C \in D_6$  be the rotation through  $\pi/3$  and  $R \in D_6$  be a reflection. We can assume  $\{Q_1, Q_1, R\} \in D_6$  with  $Q_1 = \omega_1 b_1 + \omega_2 b_2$ ,  $0 \le \omega_1, \omega_2 \le L$ . Furthermore, we can assume that the action of C and R on the basis vectors is

In conclusion, we have shown that in addition to the thirteen isomorphism classes of symmorphic two-dimensional space groups, there are four isomorphism classes of non-symmorphic groups. We have not explicitly verified that no two classes of these seventeen space groups are isomorphic, but this is easy.

From one point of view the seventeen two-dimensional space groups constitute the possible wellpaper patterns. That is, every wellpaper pattern admits one of these seventeen groups as its maximal symmetry group. Consult references [ ], [ ] for graphic illustrations of the patterns produced by each symmetry group.