elements in a column of the periodic system have properties that remain the same in the whole column, *e.g.* the number of valence electrons, and others that evolve along the column, *e.g.* the boiling point. Similarly, we found properties that remained the same in a row, *e.g.* the subgroup structure, and others that evolved along a row, *e.g.* the number of dimensions in which spontaneous magnetization or polarization is permitted.

It is a pleasure to thank Professor H. Wondratschek for his suggestions, which led to substantial improvements of the present paper.

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A Simple Characterization of the Subgroups of Space Groups*

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Abstract

The subgroups of finite index of any n-dimensional space group are determined by the solutions of a set of congruences analogous in form and meaning to the Frobenius congruences which characterize the space groups themselves. These congruences can be solved in any dimension in which the space groups are known.

Introduction

The subgroups of the space groups play a central role both in theoretical crystallography and in the interpretation of experiment. For this reason, they have been studied intensively since Hermann first discussed them fifty years ago (Hermann, 1929). Hermann singled out two classes of subgroups for special attention, those which have the same translation subgroup as the original group (translation-equivalent subgroups) and those which belong to the same geometric crystal class as the original group (class-equivalent subgroups). This is justified by Hermann's well-known theorem that *any* subgroup is a class-equivalent subgroup of a translation-equivalent subgroup.

Following Hermann, attention has been focused on finding sequences of maximal subgroups. Recently, however, it has been shown that several contemporary problems require instead a direct knowledge of the subgroups of a given (finite) index. Thus Billiet (1977, 1978) has pointed out the usefulness of a direct approach for understanding phase transitions, and this has also been shown to be effective in the theory of color symmetry, in which the k-color groups associated with a given space group are determined by its subgroups of index k (van der Waerden & Burckhardt, 1961; Senechal, 1979).

In this paper we present a simple method for finding all the subgroups of any finite index of any n-dimensional space group. It is well known (Zassenhaus, 1948; Burckhardt, 1966) that the space groups themselves are determined by the vector solutions of a set of lattice congruences called Frobenius congruences or characteristic congruences. We show that their subgroups are also determined by a set of congruences, which are completely analogous to the Frobenius congruences in form and in meaning. Thus, in principle, the subgroups can be determined in a simple way. The congruences can be solved in any dimension in which the space groups themselves are known. And since the solutions of the 'Frobenius subgroup congruences' are vectors with integer coordinates, in many cases they can quickly be found 'by hand' using the theory of linear congruences of elementary number theory.

For brevity it is assumed that the reader is familiar with elementary number theory, linear algebra and group theory, and with the space groups in two and three dimensions.

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This paper is dedicated to Professor Werner Nowacki in recognition of his fundamental contributions to mathematical crystallography.

The space groups

In this section we briefly review the principal features of the space groups which are needed in the following, and the derivation of the Frobenius congruences.

A space group G (of any dimension n) has a maximal normal Abelian subgroup T, the elements of which we identify with n-dimensional translation vectors $\mathbf{t}$ with integer coordinates. Further, the factor group G/T is isomorphic to a finite group S of isometries of n-dimensional Euclidean space E^n. Each of these isometries maps the lattice defined by T onto itself, and thus can be identified with an automorphism of T.

In order to derive the space groups G which have a given point group S, we must define multiplication in G so as to ensure that G/T will be isomorphic to S. Thus, expressing G as a union of cosets of T,

$$G = T \cup T\bar{s}_2 \cup T\bar{s}_3 \cup \ldots \cup T\bar{s}_m, \quad \bar{s}_i \longleftrightarrow s_i \in S,$$
$$i = 1, \ldots, m, \qquad \bar{s}_1 = 1, \tag{1}$$

we must have closure under coset multiplication:

$$T\bar{s}_i T\bar{s}_j = T\bar{s}_l \tag{2}$$

if, in S, $s_i s_j = s_l$. Since $T\bar{s}_i T\bar{s}_j = T(\bar{s}_i T\bar{s}_i^{-1})\bar{s}_i\bar{s}_j$, (2) requires that

(i) $\bar{s}_i T\bar{s}_i^{-1} = T$

and (ii) $T\bar{s}_i\bar{s}_j = T\bar{s}_l$.

Thus, to construct the space groups we must specify their characterizing features:

(i′) an isomorphism φ from S onto a subgroup of the group $\mathrm{Aut}(T)$ of automorphisms of T,

and a set of m^2 translations $t^*_{ij} \in T$, one for each ordered pair i, j, $1 \le i, j \le m$, such that

(ii′) $\bar{s}_i\bar{s}_j = t^*_{ij}\bar{s}_l$.

The implementation of this program is based on the theory of group extensions (Hall, 1959; Ascher & Janner, 1965). However, for the purposes of this paper it is sufficient to note that $\mathrm{Aut}(T)$ is isomorphic to the group $GL(n,Z)$ of all $n \times n$ matrices with integer coefficients and determinant ± 1; $\varphi(S)$ will be a finite subgroup of this group.

Defining two subgroups of $\mathrm{Aut}(T)$ to be equivalent if they are conjugate, we find that the same geometric point group S may have two or more inequivalent representations in $GL(n,Z)$. The corresponding space groups are then said to belong to different arithmetic crystal classes. Groups which belong to the same arithmetic class are distinguished from one another by their sets of translations t^*_{ij}, called the factor sets of the groups. (Distinct factor sets may define the same group: a space group is actually a class of groups which are conjugate under affine transformations. We assume here that a representative factor set for each class is given.) The symmorphic groups are those in which t^*_{ij} is the zero vector for every i,j; non-symmorphic groups have at least one nontrivial t^*_{ij}.

For example, the space groups $P4$ and $I4$ have the same point group, the cyclic group of order 4, $S = \{1, s, s^2, s^3\}$. However, they belong to different arithmetic classes. For $P4$, $\varphi(S)$ is generated by the matrix $(010/\bar{1}00/001)$ while for $I4$ it is generated by the inequivalent matrix $(00\bar{1}/111/0\bar{1}0)$. On the other hand, the space groups $P4$ and $P4_1$, which belong to the same arithmetic class, have different factor sets; in the latter group, if $i+j \ge 4$, $\bar{s}^i\bar{s}^j = t^*\bar{s}^{i+j(\mathrm{mod}\,4)}$, where $\mathbf{t}^* = (0,0,1)$.

A different but equivalent approach to the construction of the space groups is the following.

Each coset representative $\bar{s}_i$ in (1) can be identified with an isometry of E^n, which is, in general, a combination of a point symmetry operation and a translation. Thus $\bar{s}_i$ can be written in the form $(\boldsymbol{\tau}_i, \mathbf{s}_k)$, where $\mathbf{s}_i = \varphi(s_i)$ and $\boldsymbol{\tau}_i$ is a vector which need not have integer coordinates. In this formulation, using additive notation for vector sums, the law of coset multiplication (2) becomes

$$T(\boldsymbol{\tau}_i, \mathbf{s}_i)\, T(\boldsymbol{\tau}_j, \mathbf{s}_j) = T(\boldsymbol{\tau}_i + \mathbf{s}_i\boldsymbol{\tau}_j, \mathbf{s}_i\mathbf{s}_j) = T(\boldsymbol{\tau}_l, \mathbf{s}_l).$$

This means that $\boldsymbol{\tau}_i + \mathbf{s}_i\boldsymbol{\tau}_j = \boldsymbol{\tau}_l + \mathbf{t}^*_{ij}$, for some $t^*_{ij} \in T$, or

$$\boldsymbol{\tau}_i + \mathbf{s}_i\boldsymbol{\tau}_j - \boldsymbol{\tau}_l = \mathbf{t}^*_{ij}. \tag{3}$$

[This expression for t^*_{ij} is equivalent to that in (ii′).] We can rewrite this equation in the form

$$\boldsymbol{\tau}_i + \mathbf{s}_i\boldsymbol{\tau}_j \equiv \boldsymbol{\tau}_l \,(\mathrm{mod}\, T). \tag{4}$$

The congruences (4) are known as Frobenius, or characteristic, congruences; each space group is completely characterized (up to affine equivalence) by the solution set $\{\boldsymbol{\tau}\}$ and by the isomorphism φ.

If S has w generators $u_1, u_2, \ldots, u_w$ which satisfy r defining relations $R_i(u_1, u_2, \ldots, u_w) = 1$, $i = 1, \ldots, r$, then the Frobenius congruences imply the r congruences

$$R_i(\bar{u}_1, \bar{u}_2, \ldots, \bar{u}_w) \equiv 0 \;(\mathrm{mod}\, T) \tag{5}$$

and conversely. Since, in general, $r < m^2$, it is often convenient to use (5) instead of (4).

The congruences (4) and (5) were used by Zassenhaus and Burckhardt as the basis for algorithms for constructing the space groups. An interesting geometric interpretation of Zassenhaus's theorem was given by Galiulin (1969), who carried out the Zassenhaus algorithm for $n = 3$. (See also Brown, 1969.) Recently, the characterization and enumeration of the four-dimensional space groups were completed by Brown, Bülow, Neubüser, Wondratschek & Zassenhaus (1978).

Subgroups

The following version of Hermann's theorem can be established without difficulty (see Senechal, 1979).

Theorem 1

Let G be an n-dimensional space group with arithmetic class S and translation subgroup T. If H is a subgroup of G of finite index k, then

(i) $T' = H \cap T$ is a maximal Abelian normal subgroup of H,

(ii) H/T' is isomorphic to a subgroup S' of S, and thus H can be written as a union of cosets of T':

$$H = \bigcup_i T'\bar{\bar{s}}_i', \quad \bar{\bar{s}}_i' \longleftrightarrow s_i' \in S',$$

and

(iii) the index of H in G is given by the formula

$$k = [G:H] = [S:S'][T:T'] = \mu\Delta.$$

If $\Delta = 1$, H is a translation-equivalent subgroup of G; if $\mu = 1$, H is a class-equivalent subgroup.

Thus, in order to find the subgroups of index k of G, we must know the subgroups S' of S of index μ, for each divisor μ of k. Our task is then to find the class-equivalent subgroups of the translation-equivalent subgroup with arithmetic class S'. To do this, we look for subgroups T' of index $k/\mu = \Delta$ and coset representatives $\bar{\bar{s}}_i' \in G$ such that the cosets $T'\bar{\bar{s}}_i'$ form a group isomorphic to S'.

Since T' will be a subgroup of T, we can write

$$T = T' \cup T't_2 \cup \ldots T't_\Delta.$$

Then we have, from (1),

$$G = \bigcup_i \bigcup_j T't_i\bar{s}_j. \qquad (6)$$

This tells us that the coset representatives $\bar{\bar{s}}'$ have the form $\bar{\bar{s}}' = t\bar{s}'$, or, in the alternative notation, $(\mathbf{t} + \boldsymbol{\tau}', \mathbf{s}')$.

It is easy to show that if the union of a subset of the cosets of T' in (6) is a subgroup H with $H/T' = S'$, then any two elements of the form $t_1\bar{s}$ and $t_2\bar{s}$ must belong to the same coset of T'. Thus we can index the cosets $T't_i\bar{s}_i'$, $i = 1, \ldots, m/\mu$, where, as before, m is the number of elements in S.

The set of cosets must be closed under multiplication and so, when $s_i's_j' = s_l'$ in S', we have

$$(T't_i\bar{s}_i')(T't_j\bar{s}_j') = T't_l\bar{s}_l'.$$

In order for this equality to hold, we must have, in analogy with (i) and (ii) of (2),

(iii) $\bar{s}_i'T'\bar{s}_i'^{-1} = T'$,

(iv) $T'(t_i\bar{s}_i't_j\bar{s}_j') = T'(t_l\bar{s}_l')$.

Thus each $\varphi(s_i')$ must be an automorphism of T'. Further, writing each $t\bar{s}'$ in the form $(\mathbf{t} + \boldsymbol{\tau}', \mathbf{s}')$, (iv) becomes

$$\begin{aligned} T'(\mathbf{t}_i + \boldsymbol{\tau}_i', \mathbf{s}_i')(\mathbf{t}_j + \boldsymbol{\tau}_j', \mathbf{s}_j') &= T'(\mathbf{t}_i + \boldsymbol{\tau}_i' + \mathbf{s}_i'\mathbf{t}_j + \mathbf{s}_i'\boldsymbol{\tau}_j', \mathbf{s}_i'\mathbf{s}_j') \\ &= T'(\mathbf{t}_l + \boldsymbol{\tau}_l', \mathbf{s}_l'), \end{aligned}$$

which implies that

$$\mathbf{t}_i + \boldsymbol{\tau}_i' + \mathbf{s}_i'\mathbf{t}_j + \mathbf{s}_i'\boldsymbol{\tau}_j' \equiv \mathbf{t}_l + \boldsymbol{\tau}_l' (\text{mod } T')$$

or

$$(\boldsymbol{\tau}_i' + \mathbf{s}_i'\boldsymbol{\tau}_j' - \boldsymbol{\tau}_l') + \mathbf{t}_i + \mathbf{s}_i'\mathbf{t}_j \equiv \mathbf{t}_l (\text{mod } T').$$

Since, by (3), the expression in parentheses is equal to $\mathbf{t}_{ij}^{*\prime}$, we obtain the subgroup analogue of (3),

$$\mathbf{t}_{ij}^{*\prime} + \mathbf{t}_i + \mathbf{s}_i'\mathbf{t}_j \equiv \mathbf{t}_l (\text{mod } T'). \qquad (7)$$

If any of the vectors $\mathbf{t}$ in (7) is replaced by $\mathbf{t} + \mathbf{t}'$, $\mathbf{t}' \in T'$, the congruence is unchanged. Thus two vectors whose difference lies in T' define the same subgroup; a solution of (7) is understood to be a solution modulo T'. Since any vector outside (or on a face) of a primitive cell of the sublattice of T' is congruent modulo T' to a vector inside or on the opposite face of the cell, and since there are Δ lattice points per cell, the number of possibilities for t does not exceed Δ.

Since G is a known space group, the vectors $\mathbf{t}_{ij}^*$ and the operations $\mathbf{s}_i$ are known. Thus the subgroups of G with $H/T' = S'$ are determined by the vector solutions $\mathbf{t}_i, \mathbf{t}_j, \mathbf{t}_l$.

Theorem 2. *The Frobenius subgroup theorem*

Let $G = \bigcup_{i=1}^m T(\tau_i, \mathbf{s}_i)$ be a space group with point group S of order m, arithmetic crystal class $\varphi(S)$, translation subgroup T and factor set $\{t_{ij}^*\}$. Each subgroup H of finite index k of G is determined by a pair of subgroups $T' \subseteq T$ and $S' \subseteq S$, where $[S:S'][T:T'] = k = \mu\Delta$. Further,

$$H = \bigcup_{l=1}^{m/\mu} T'(\mathbf{t}_l + \boldsymbol{\tau}_l', \mathbf{s}_l'),$$

where $t_l \in T$ and, for $s_l' \in S'$,

$$\mathbf{s}_l' = \varphi(s_l').$$

S' and T' are constrained by the conditions

(i) $\varphi(S') \subset \text{Aut}(T')$,

and

(ii) $\mathbf{t}_{ij}^{*\prime} + \mathbf{t}_i + \mathbf{s}_i'\mathbf{t}_j \equiv \mathbf{t}_l (\text{mod } T')$

when $s_i's_j' = s_l'$ in S'.

We note that these congruences can be replaced by an equivalent set involving the generators of S', analogous to (5).

Examples

In order to find all the subgroups of index k of a given space group G, we consider all possible products $\mu\Delta =$

k, and follow the steps implicit in the preceding discussion:

(1) find all subgroups S' of S of index μ;

(2) for each subgroup S', find all subgroups T' of T of index Δ which are invariant under the operations $\varphi(S')$;

(3) solve the congruences (7) or an equivalent set. The solutions will be sets of vectors with integer coordinates.

Step 1 is straightforward in those dimensions in which the space groups are known. To carry out step 2, we observe that each sublattice of the lattice defined by T is generated by a set of n basis vectors $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_n$ with integer coordinates. These n vectors form the columns of a matrix $A = [a_{ij}]$ with integer entries; $[T:T'] = \Delta = \det A$. (Square brackets are used to emphasize the fact that in this context A is not intended to be a linear transformation.) A different choice of basis would result in a different matrix B, which is related to A by the equation $B = AX$, where X is an $n \times n$ matrix with integer entries and determinant ± 1, *i.e.* an element of $GL(n,Z)$. (The product AX is formed by ordinary matrix multiplication.) In view of this, we see that T' is invariant under the motions $\varphi(s')$, $s' \in S'$, if for each s', $\varphi(s')$ maps A onto itself or onto another basis for T', that is, if there exists an X such that $\mathbf{s}'A = AX$. This equation places arithmetic constraints on the coordinates of the vectors $\mathbf{a}_i$, which thus define a finite set of possible forms for the matrix A. (The distinct forms of the set are rationally equivalent; that is, they are conjugate in the group of all matrices with rational entries.) It should be noted that since the forms of the matrices are completely determined by the motions $\varphi(s')$, this set is the same for all groups belonging to the same arithmetic crystal class. [In this paper we will not derive these forms; for details see Harker (1978) and Senechal (1979).] Finally, to complete step 3, we solve the appropriate vector congruences. If there is more than one form for the matrix A, each must be considered separately.

We illustrate these steps by characterizing the subgroups of finite index k of the plane group $p4$ and the three-dimensional space groups $P4$ and $P4_1$.

Step 1. For all three groups, S is cyclic of order 4, generated by a single element s satisfying the relation $s^4 = 1$. The subgroups S' of S are $S_1 = \{1\}$, $S_2 = \{1,s^2\}$ and $S_3 = S = \{1,s,s^2,s^3\}$. Thus these groups can have subgroups of indices $k = 4\Delta$, $k = 2\Delta$, and $k = \Delta$; the possible values of Δ are discussed below.

Step 2. If $S' = S_1$ then the subgroup H is simply T' itself. Since $\varphi(S')$ contains only the identity automorphism, any matrix A with $\det A = k/4$ is admissible. Thus for $p4$ the matrix form is the general $[pq/st]$ and for $P4$ and $P4_1$, its 3×3 analogue.

If $S' = S_2$, the lattices must be invariant under a twofold rotation. Every planar lattice satisfies this requirement, so for $p4$ the matrix A has the general form above. For $P4$ and $P4_1$, we have (Harker, 1978) two forms corresponding to the monoclinic primitive lattice, MP, $[pq0/st0/00r]$, and to the monoclinic centered lattice, MC, $[pqr/\bar{p}\bar{q}r/st0]$.

If $S' = S_3 = S$, then the lattices must be invariant under a fourfold rotation. In this case the matrix for the plane lattice can be written in the form $[pq/\bar{q}p]$, with $\Delta = p^2 + q^2$. The three-dimensional tetragonal lattices can be primitive, SP, $[pq0/\bar{q}p0/00r]$ or centered, SI, $[pqr/\bar{q}pr/\bar{p}\bar{q}r]$. Their determinants are $r(p^2 + q^2)$ and $2r(p^2 + q^2)$, respectively.

Table 1. *The subgroups of* $P4$ *and* $P4_1$

If G is one of the space groups $P4$ and $P4_1$, then G/T is isomorphic to a cyclic group S of order 4, and the group of automorphisms $\varphi(S)$ is generated by the transformation $\mathbf{s} = (010/\bar{1}00/001)$. The subgroups of G are determined by the subgroups $S' \subseteq S$, the appropriate sublattices $T' \subseteq T$, and the corresponding vector congruences. The solutions are elements of T, that is, they are vectors with integer coordinates. (Thus, in columns 4 and 5 it is understood that the stated solution exists only when r is divisible as indicated.)

Generator of $\varphi(S')$	Congruence (mod T')	Matrix for T'	$P4$ Solutions $\mathbf{t}$	$P4$ Subgroup type	$P4_1$ Solutions $\mathbf{t}$	$P4_1$ Subgroup type
I_3	–	$[pqr/stu/vw0]$	(x,y,z)	$P1$	(x,y,z)	$P1$
$(\bar{1}00/0\bar{1}0/001)$	$\mathbf{t}^* + \mathbf{t} + \mathbf{s}^2\mathbf{t} = \mathbf{0}$	$[pq0/st0/00r]$	$(x,y,0)$	$P2$	$[x, y, (r-1)/2]$	$P2_1$
			$(x,y,r/2)$	$P2_1$		
		$[pqr/\bar{p}\bar{q}r/st0]$	$(x,y,0)$	$C2$	–	
			(x,y,r)	$C2$		
$(010/\bar{1}00/001)$	$\mathbf{t}^* + \bigcup_{i=0}^{3} \mathbf{s}^i\mathbf{t} \equiv \mathbf{0}$	$[pq0/\bar{q}p0/00r]$	$(x,y,0)$	$P4$	$[x, y, (r-1)/4]$	$P4_1$
			$(x,y,r/2)$	$P4_2$	$[x, y, (3r-1)/4]$	$P4_3$
			$(x,y,r/4)$	$P4_1$		
			$(x,y,3r/4)$	$P4_3$		
		$[pqr/\bar{q}pr/\bar{p}\bar{q}r]$	$(x,y,0)$	$I4$	–	
			(x,y,r)	$I4$		
			$(x,y,r/2)$	$I4_1$		
			$(x,y,3r/2)$	$I4_1$		

Step 3. Whenever S' is the identity subgroup S_1, (7) is satisfied trivially. Each lattice of determinant $k/4$ defines a subgroup of T of index k. For example, if $k = 20$, $p4$ has exactly six subgroups of this type, described by the matrices $[50/j1], j = 0, \ldots, 4$ and $[10/05]$.

When $S' = S_2$, $H = T' \cup T't\bar{s}^2$ for some $t \in T$. The subgroup S_2 has two elements so there will be four congruences (7). However, since three of them involve the identity automorphism, only the one in which both s_i and s_j are equal to s^2 needs to be solved:

$$\mathbf{t}^* + \mathbf{t} + \mathbf{s}^2\mathbf{t} \equiv \mathbf{0}(\text{mod } T'). \tag{8}$$

When $G = p4$, $\mathbf{s}^2 = -I_2$ and $\mathbf{t}^* = (0,0)$. Thus (8) is satisfied by any $t \in T$. *When* $G = P4$, then again the subgroups with $S' = S_2$ are determined by the solutions of the congruence (8), where T' is given by one of the lattices MP or MC, $\mathbf{t}^* = (0,0,0)$ and $\varphi(s^2) = (\bar{1}00/0\bar{1}0/001)$. Writing $\mathbf{t} = (x,y,z)$, (8) becomes

$$(x,y,z) + (-x,-y,z) \equiv (0,0,0)(\text{mod } T').$$

This means that the vector $(0,0,2z)$ must be an integral multiple of the shortest vector in T' in the direction $[0,0,1]$. In the MP lattice, this vector is $(0,0,r)$; in the MC lattice it is $(0,0,2r)$. Thus to find the solutions $\mathbf{t}$ we must solve the arithmetic congruences $2z \equiv 0(\text{mod } r)$ and $2z \equiv 0(\text{mod } 2r)$, respectively. The first congruence always has the solution $z = 0$; thus any vector $(x,y,0)$ is a solution of (8). The subgroups they determine are of type $P2$. If r is even $[2|r]$, then there is the additional solution $z = r/2$; thus (8) is satisfied by all vectors of the form $\mathbf{t} = (x,y,r/2)$. These subgroups are of type $P2_1$. The second congruence always has two solutions, $z = 0$ and $z = r$; both determine subgroups of type $C2$. *When* $G = P4_1$, (8) becomes

$$(0,0,1) + (0,0,2z) \equiv (0,0,0)(\text{mod } T')$$

which reduces to the two congruences $2z+1 \equiv 0(\text{mod } r)$ and $2z+1 \equiv 0(\text{mod } 2r)$, according as T' has an MP or MC lattice. The first congruence has no solution for even values of r. For odd r $[2|(r-1)]$, there is the unique solution $z = (r-1)/2$; the corresponding subgroups are of type $P2_1$. The second congruence has no solutions for any r.

Finally, when $S' = S_3 = S$, then $H = \cup_{i=1}^{4}(T't\bar{s})^{i-1}$; in this case it is convenient to replace the congruences (7) by the single congruence determined by the relation $(T't\bar{s})^4 = T'$:

$$\mathbf{t}^* + \mathbf{t} + \mathbf{s}\mathbf{t} + \mathbf{s}^2\mathbf{t} + \mathbf{s}^3\mathbf{t} \equiv \mathbf{0}(\text{mod } T'). \tag{9}$$

When $G = p4$, there are no subgroups unless Δ is an integer which can be written as a sum of two squares. (The number of lattices is a function of the number of ways in which this can be done.) Since $\mathbf{t}^* = (0,0)$ and the group $\varphi(S)$ is generated by $(01/\bar{1}0)$, (9) becomes

$$(x,y) + (-y,x) + (-x,-y) + (y,-x) \equiv (0,0)(\text{mod } T'),$$

where $(x,y) = \mathbf{t}$. This congruence is satisfied by all vectors $\mathbf{t}$. The subgroups of this type of index 5 are illustrated in Fig. 1. *When* $G = P4$, (9) becomes

$$(x,y,z) + (-y,x,z) + (-x,-y,z) + (y,-x,z) \equiv (0,0,0)(\text{mod } T').$$

For the SP lattice, this reduces to $4z \equiv 0(\text{mod } r)$. This congruence always has the solution $z = 0$, so $\mathbf{t} =$

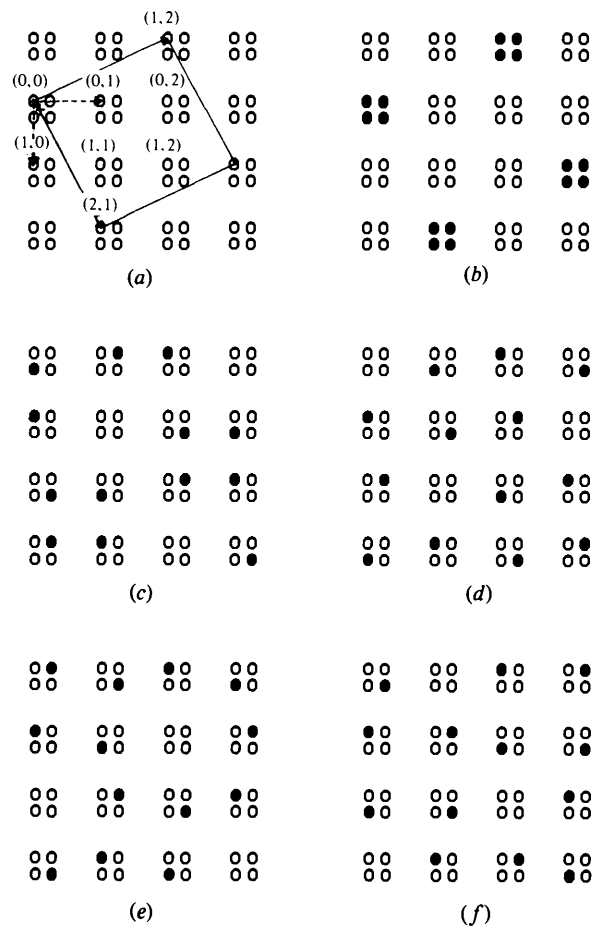

Fig. 1. The subgroups of index 5 of the plane group $p4$ with sublattice $[21/\bar{1}2]$, represented by their orbits. (An orbit for a group of motions is the set of points generated from an arbitrary point by those motions.) (*a*) An orbit (with points in general position) for the plane group $p4$. The initial point is $(0,0)$; the center of the rotation $\mathbf{s}$ is marked by a +. A subgroup of $p4$ of index k with $\mu = 1$, $\Delta = k$ is also type $p4$; the sublattice matrix must have the form $[pq/\bar{q}p]$. If $k = 5$, there are two possible lattices, $[21/\bar{1}2]$ and $[2\bar{1}/12]$. A primitive cell of the sublattice defined by the first of these is shown. (*b*) A subgroup of $p4$ corresponds to each distinct solution of the congruence $\cup_{i=0}^{3}\mathbf{s}^i\mathbf{t} \equiv 0(\text{mod } T')$. If T' is defined by the matrix $[21/\bar{1}2]$ then the vector $\mathbf{t} = (0,0)$ and the vectors lying inside the primitive cell are the five distinct solutions. The orbit of the subgroup defined by the solution $\mathbf{t} = (0,0)$ is indicated by filled circles. (*c*)–(*f*) The orbits of the subgroups defined by the solutions $\mathbf{t} = (1,1)$, $\mathbf{t} = (1,2)$, $\mathbf{t} = (0,1)$ and $\mathbf{t} = (0,2)$, respectively. In each case the starting point of the orbit is the point $(0,0)$ of (*a*). Computer drawing programmed by Lynn Goodhue.

$(x,y,0)$ is always a solution of (9). The corresponding subgroups are of type $P4$. If $2|r$, then $z = r/2$ is also a solution and the corresponding vector solutions of (9), $\mathbf{t} = (x,y,r/2)$, determine $P4_2$ subgroups. Finally, if $4|r$, there are $P4_1$ subgroups corresponding to the solution $z = r/4$ and $P4_3$ subgroups corresponding to the solution $z = 3r/4$. For the SI lattice the congruence reduces to $4z \equiv 0 \pmod{2r}$. There are always the solutions $z = 0$ and $z = r$, to which correspond subgroups of type $I4$. If $2|r$ then there are also $I4_1$ subgroups corresponding to the additional solutions $z = r/2$ and $z = 3r/2$. *When* $G = P4_1$, (9) becomes

$$(0,0,1) + (0,0,4z) \equiv (0,0,0)(\mathrm{mod}\ T'),$$

which reduces to $4z + 1 \equiv 0 \pmod{r}$ and $4z + 1 \equiv 0 \pmod{2r}$. The second has no solutions. The first has no solutions if $2|r$, and has the unique solution $z = (r-1)/4$ if $4|(r-1)$ and $z = (3r-1)/4$ if $4|(r-3)$. The subgroup is $P4_1$ in the first case and $P4_3$ in the second. The defining characteristics of the subgroups of $P4$ and $P4_1$ are listed in Table 1.

Concluding remarks

In many problems we need to be able to classify the subgroups of a space group G; the definition of equivalence depends upon the problem at hand. Most generally, two subgroups are equivalent if one can be mapped onto the other by an automorphism of G. However, in some problems we may need to distinguish further between sense-preserving and sense-reversing automorphisms, or between inner and outer automorphisms. The equivalence problem will not be discussed here; for detailed discussions we refer the reader to Opechowski (1980) and Senechal (1979).

The characterization of the subgroups presented in this paper complements other recent work in this field. Köhler (1980*a*,*b*,*c*) discusses both the periodic crystallographic groups (*i.e.* n-dimensional space groups and crystallographic point groups) and subperiodic groups (groups in which the translation subgroup has lower dimension than the group) from a unified abstract point of view. A generalization of Zassenhaus's algorithm is used to construct these groups and to characterize their subgroups. For the periodic groups his results are in accordance with ours. In several papers, Billiet and his colleagues have discussed the problem of determining whether one space group g can be a subgroup of another G (*e.g.* Billiet, Sayari & Zarrouk, 1978). They show that it is necessary that the point group of g be a subgroup of the point group of G, and that it must be possible to identify an orbit of g (see the caption to Fig. 1) as a suborbit of an orbit of G. In our terminology, this means that $S' \subseteq S$ and T' must be a sublattice of T invariant under the automorphisms $\varphi(S')$; thus their approach to subgroups is also closely related to that presented here. Recently, Bertaut & Billiet (1979) have shown that the fact that the subgroups which are isomorphic to G are also affine conjugate to it can be used in their determination.

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