Acta Crystallographica Section A
Foundations of Crystallography
ISSN 0108-7673

Received 19 July 2005
Accepted 18 November 2005

Some algebraic properties of crystallographic sublattices

John S. Rutherford

National University of Science and Technology, Bulawayo, Zimbabwe. Correspondence e-mail: john.rutherford9@btinternet.com

In this article, a number of the results relevant to the concept of sublattices of a basic crystallographic lattice are reviewed, emphasizing particularly previously unpublished work on the algebraic aspects. A three-dimensional geometric lattice $\boldsymbol{L}$ can be considered as an infinite Abelian group under addition. A sublattice $\boldsymbol{S}$ of $\boldsymbol{L}$, which is also three-dimensional, is a subgroup of $\boldsymbol{L}$ such that the finite quotient group,

$$G \simeq \boldsymbol{L}/\boldsymbol{S},$$

is an Abelian group of order the index of $\boldsymbol{S}$ in $\boldsymbol{L}$. The sublattice itself in its standard form is represented by an upper triangular matrix. The index of the sublattice is given by the determinant of this matrix. It is first noted that a sublattice described by an arbitrary basis set in $\boldsymbol{L}$ may be converted to this standard form. Next the sublattice is expressed as the intersection of a set of sublattices of individual index a power of a distinct prime, *i.e.*

$$\boldsymbol{S}(n = p_1^a p_2^b \ldots) = \boldsymbol{S}_1(p_1^a) \cap \boldsymbol{S}_2(p_2^b) \cap \ldots = \bigcap_i \boldsymbol{S}_i(p_i^{\alpha_i}),$$

where p_1, p_2 *etc.* are prime numbers and $n = \prod_i p_i^{\alpha}$ is the Euclidean factorization of n. This decomposition is important because it corresponds to the Sylow decomposition of the corresponding quotient group

$$G \cong \bigotimes_i A_{p_i}.$$

It is also useful to be able to carry out two commutative binary operations on sublattices of $\boldsymbol{L}$; these are to find their common sublattice of lowest index in $\boldsymbol{L}$, which is their intersection

$$\boldsymbol{S}_{\cap} = \boldsymbol{S}_a(m) \cap \boldsymbol{S}_b(n)$$

and their common superlattice of highest index in $\boldsymbol{L}$, given by

$$\boldsymbol{S}_{<>} = \langle \boldsymbol{S}_a(m), \boldsymbol{S}_b(n) \rangle,$$

where <> indicates the span of the sublattices.

1. Introduction

The concept of a sublattice of a basic crystallographic lattice in two or three dimensions is crucial to the many applications of group–subgroup relations in crystallography and, although much is known regarding sublattices in general (Conway & Sloane, 1988), more could be done to make this knowledge available to practising crystallographers. In addition, the whole subject is clouded by a confusion in terminology; a lattice that contains only a fraction of the points of the basic lattice defining the system, properly called a sublattice, is frequently referred to as a (commensurate) superlattice, or as a derivative lattice. Although much presented here applies to such sublattices in an abstract sense, for the purposes of the suggested applications we shall consider the basic lattice to typically represent an ideal or average crystal structure, on which is imposed a periodic disturbance in position, composition or magnetic properties, such that only points of the sublattice are truly identical by translation to the common origin of both lattices.

In this article, we review a number of the relevant results, emphasizing particularly previously unpublished work on the algebraic aspects, since the number-theory-based enumerative methods have recently been summarized elsewhere (Rutherford, 2003).

For convenience, we shall focus on three-dimensional lattices here. Such a geometric lattice $\boldsymbol{L}$ can be considered as an infinite Abelian group under addition. A sublattice $\boldsymbol{S}$ of $\boldsymbol{L}$

which is also three-dimensional is a subgroup of $\boldsymbol{L}$ under addition, such that the quotient group

$$G \cong \boldsymbol{L}/\boldsymbol{S} \tag{1}$$

is a finite Abelian group of order $|G| = [\boldsymbol{L} : \boldsymbol{S}]$ (*i.e.* the order of G is the index of $\boldsymbol{S}$ in $\boldsymbol{L}$). When $|G|$ is the natural number n, the structure of the group G is restricted by the number of dimensions of the lattice to the direct product of at most three cyclic groups and, because of the fundamental theorem on the structure of such finite Abelian groups (Lang, 2002), its structure may be expressed in the form

$$G \cong C_a \otimes C_b \otimes C_c, \tag{2}$$

where $n = abc$, $c|b$ (*i.e.* c is a divisor of b), and $b|a$. According to the classification of Harker (1978), if $c \neq 1$ then G is of type I, if $c = 1$ and $b \neq 1$ it is of type II and if $b = c = 1$ then it is of type III.

For example, if G has order 72, it must be one of

type I: $C_6 \otimes C_6 \otimes C_2$ or $C_{18} \otimes C_2 \otimes C_2$
type II: $C_{12} \otimes C_6$ or $C_{24} \otimes C_3$ or $C_{36} \otimes C_2$
type III: C_{72}.

Now, if the sublattice represents the period of a perturbation of an underlying crystal structure in $\boldsymbol{L}$, each cycle in the structure of G must correspond to an independent vector of this perturbation. Each such propagation vector is formally represented by an additional dimension when the period of the perturbation is incommensurate with $\boldsymbol{L}$. So, using this analogy, a type III sublattice, for example, is comparable to a (3 + 1) dimensionality in the incommensurate case.

Turning to the sublattices themselves, these are characterized by three independent vectors of $\boldsymbol{L}$. In general, there are an infinite number of ways to define the unit cell of the sublattice, but each sublattice can be expressed in, for example, the Hermite normal form (Cohen, 1993) as chosen by Billiet & Rolley-Le Coz (1980) as standard. Here the sublattice is represented by an upper triangular matrix, which generates the basis vectors of the sublattice by post-multiplication on the basis vectors of $\boldsymbol{L}$. The index of the sublattice is given by the determinant of this matrix, *i.e.* (abc) in the example below:

$$\begin{pmatrix} a & d & e \\ 0 & b & f \\ 0 & 0 & c \end{pmatrix}. \tag{3a}$$

Billiet & Rolley-Le Coz (1980) chose a particular option for the off-diagonal elements of the matrix which requires d and e to lie in the range

$$\begin{aligned} &-(a-1)/2, -(a-1)/2+1, \ldots, (a-1)/2-1, (a-1)/2 \quad && a \text{ even}, \\ &-a/2+1, -a/2+2, \ldots, a/2-1, a/2 && a \text{ odd}, \end{aligned} \tag{3b}$$

and f to lie in the equivalent range with respect to b.

Fig. 1 shows for a two-dimensional sublattice a possible conventional or reduced cell and the corresponding standard cell choice.

The ranges stated in (3b) mean that, for an index n with a specific set of divisors a, b and c, there are a possible values for each of d and e, and b possible values for f, giving a^2b in all.

It is also possible to transform the matrix above by standard matrix operations to a diagonal form, the Smith or elementary

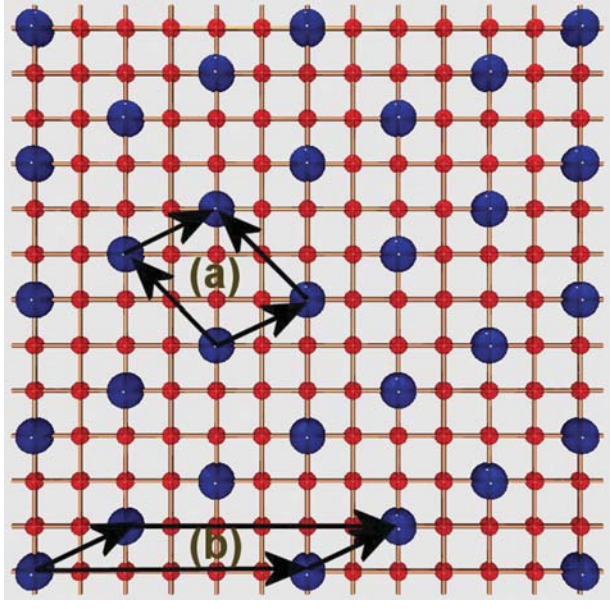

Figure 1
A sublattice (blue spheres) of a basic crystallographic lattice in two dimensions (red and blue spheres). (*a*) A possible convention or reduced cell. (*b*) The standard cell choice.

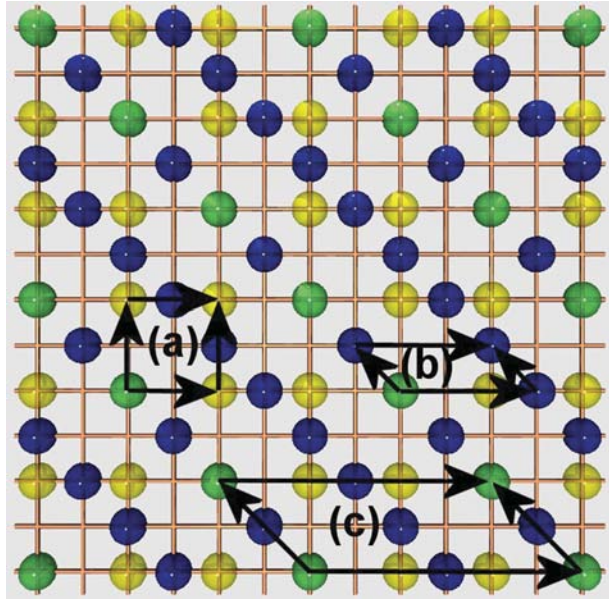

Figure 2
The construction of a sublattice from the intersection of sublattices with prime-power indices. (*a*) Unit cell of sublattice ($2\ 0/0\ 2$) index 4, yellow and green spheres. (*b*) Unit cell of sublattice ($3\ \bar{1}/0\ 1$) index 3, blue and green spheres. (*c*) Unit cell of their intersection ($6\ \bar{2}/0\ 2$), index 12, green spheres.

divisor normal form (Cohen, 1993), which shows the structure of G explicitly.

2. Sublattice algebra

Now it has been shown that the set of sublattices of $\boldsymbol{L}$ are multiplicative in the primes (Rutherford, 1992; Gruber, 1997). That means there is a distinct sublattice $\boldsymbol{S}(mn)$ of index (mn) corresponding to each distinct $\boldsymbol{S}_a(m)$ and $\boldsymbol{S}_b(n)$, when m and n are mutually prime, *i.e.* when their greatest common divisor, written (m, n), is 1. This sublattice is, in fact, given by

$$\boldsymbol{S}(mn) = \boldsymbol{S}_a(m) \cap \boldsymbol{S}_b(n). \tag{4}$$

When m and n contain a common divisor, not only does equation (4) no longer apply but the intersection $\boldsymbol{S}(\mu|mn) = \boldsymbol{S}_a(m) \cap \boldsymbol{S}_b(n)$ may arise in more than one way, in the sense that

$$\boldsymbol{S}_a(m) \cap \boldsymbol{S}_b(n) = \boldsymbol{S}_c(m) \cap \boldsymbol{S}_d(n)$$

becomes a possibility.

The source of the multiplicative property is the fact that we can express each sublattice as the intersection of a set of sublattices of individual index a power of a distinct prime, *i.e.*

$$\boldsymbol{S}(n = p_1^a p_2^b \ldots) = \boldsymbol{S}_1(p_1^a) \cap \boldsymbol{S}_2(p_2^b) \cap \ldots = \bigcap_i \mathbf{S}_i(p_i^{\alpha_i}), \tag{5}$$

where p_1, p_2 *etc.* are prime numbers and $n = \prod_i p_i^{\alpha_i}$ is the Euclidean factorization of n. For example, we thus show in Fig. 2

$$\begin{pmatrix} 6 & 3 \\ 0 & 2 \end{pmatrix} = \begin{pmatrix} 2 & 1 \\ 0 & 2 \end{pmatrix} \cap \begin{pmatrix} 3 & 0 \\ 0 & 1 \end{pmatrix}.$$

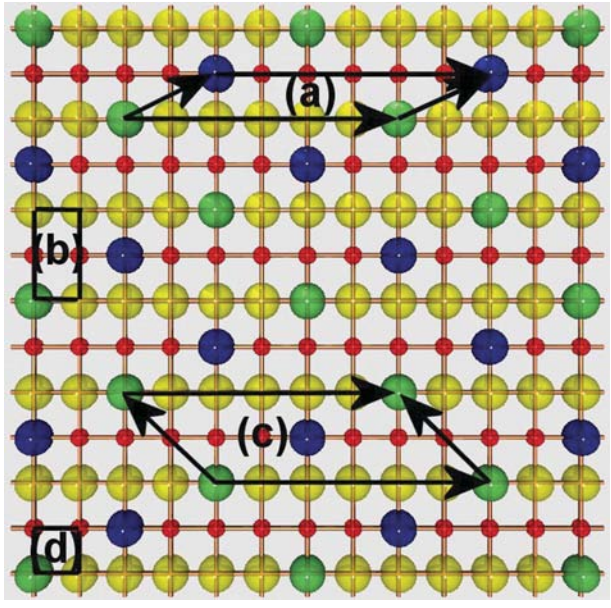

Figure 3
Binary operations, $\boldsymbol{S}_{<>} = \boldsymbol{L}$ case. (*a*) Sublattice 1 (blue and green). (*b*) Sublattice 2 (yellow and green). (*c*) Their intersection (green only). (*d*) Their sum (red, blue, yellow and green).

This decomposition is important because it corresponds to the Sylow decomposition (Lang, 2002) of G,

$$G \cong \bigotimes_i A_{p_i}, \tag{6}$$

where each group A_{p_i} is of order $p_i^{\alpha_i}$, each $A_{p_i} \subseteq G$, and α_i is the highest possible power of p_i, *i.e.* p_i does not divide $[G : A_{p_i}]$. The groups A_{p_i} are then the p-Sylow subgroups of G.

Now, because the structures of the p-Sylow subgroups are not simple direct products, we cannot properly carry the decomposition process beyond the prime power lattices $\boldsymbol{S}(p_i^{\alpha_i})$. As a simple example of the problems that arise, consider the group structures of the Abelian groups of order p^2, p prime. These are C_{p^2} and $C_p \otimes C_p$. C_{p^2} has only one subgroup of order p, while $C_p \otimes C_p$ has $(p + 1)$. If we take the intersection of two distinct sublattices of index p, we get

$$\boldsymbol{S}_{ab}(p^2) = \boldsymbol{S}_a(p) \cap \boldsymbol{S}_b(p), \quad \boldsymbol{S}_a \neq \boldsymbol{S}_b,$$

where $G(\boldsymbol{S}_{ab}) \cong C_p \otimes C_p$. Each possible $\boldsymbol{S}_{ab}$ may be constructed from any of a large number of pairs of sublattices of individual index p, while, on the other hand, it is impossible to construct a sublattice with quotient group C_{p^2} as the intersection of two such sublattices.

One potential application of sublattices is the enumeration of possible structures based on two or more motifs occupying cells of a basic lattice by the Polya method (Polya & Read, 1987). To do this for the complete set of sublattices of index n, as in Rutherford (1995), we need only enumerate the sublattices of each possible group structure, using the appropriate formulae (Rutherford, 1993). On the other hand, if we wish to find the possible structures corresponding to a specific sublattice, we apply the Smith normal form to assign its quotient group structure G.

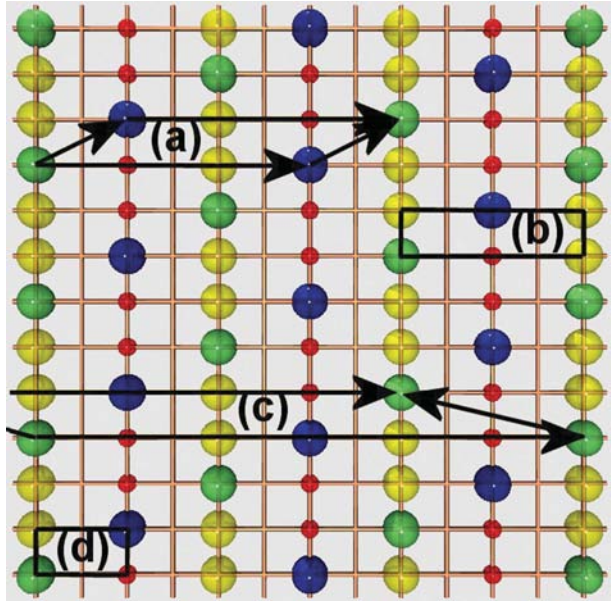

Figure 4
As Fig. 3 but for the $\boldsymbol{S}_{<>} \neq \boldsymbol{L}$ case.

Further, we wish to be able to carry out two commutative binary operations on sublattices of $\boldsymbol{L}$; these are to find their common superlattice of highest index in $\boldsymbol{L}$, given by

$$\boldsymbol{S}_{<>} = \langle \boldsymbol{S}_a(m), \boldsymbol{S}_b(n) \rangle, \tag{7}$$

where <> indicates the span of the sublattices, and their common sublattice of lowest index in $\boldsymbol{L}$, which is their intersection

$$\boldsymbol{S}_{\cap} = \boldsymbol{S}_a(m) \cap \boldsymbol{S}_b(n). \tag{8}$$

The relevance of these operations lies in the various applications of space-group–subgroup relations in crystallography. The lattice–sublattice relation corresponds to an equiclass relation between space groups, one of the two possible components of a general space-group–subgroup relation, the other being the equitranslational component. So, throughout the remainder of this section, we shall call the space group of the highest symmetry crystal structure in our tree of space-group–subgroup relations – the aristotype in Bärnighausen's (1980) terminology – K, and apply the notation $\boldsymbol{S}(H)$ to imply the sublattice of $\boldsymbol{L}(K)$ which corresponds to the subgroup of translations of the space group $H \subset K$. We first note that, if we have two such space groups $H \subset K$, there is an important intermediate space group, the Hermann group M, of profound practical importance (Wondratschek & Aroyo, 2001), such that

$$H \subseteq M \subseteq K$$

with H an equiclass subgroup of M, and the lattice of $\boldsymbol{S}(H)$ is a sublattice of index $[M:H]$ of the common lattice $\boldsymbol{L}$ of M and K. In addition, we may find, for two such subgroups H_1 and H_2 of K, by applying $\boldsymbol{S}_{<>}$ to $\boldsymbol{S}(H_1)$ and $\boldsymbol{S}(H_2)$, the lattice of their minimal common supergroup, an important step in the construction of Bärnighausen (1980) trees, and, by applying $\boldsymbol{S}_{\cap}$, the lattice of their maximal common subgroup, which may likewise be an aid in applying the Stokes & Hatch (2002) approach to the mechanism of discontinuous phase transitions.

We can examine the possible indices of $\boldsymbol{S}_{\cap}$ and $\boldsymbol{S}_{<>}$ using relationship (5). Writing m for $[M_1:H_1]$ and n for $[M_2:H_2]$, we have

$$\boldsymbol{S}_a(m) = \bigcap_i \mathbf{S}_a(p_i^{\alpha_i}), \quad m = \prod_i p_i^{\alpha_i} \tag{9a}$$

and

$$\boldsymbol{S}_b(n) = \bigcap_i \mathbf{S}_b(p_i^{\beta_i}), \quad n = \prod_i p_i^{\beta_i}. \tag{9b}$$

For a specific p_i, the factor of the largest common divisor (m,n) will be $p_i^{\gamma_i}$, where γ_i is the lesser of α_i and β_i, and hence $(m,n) = \prod_i p_i^{\gamma_i}$.

So $A_{p_i}(<>)$ the p-Sylow subgroup of $G(S_{<>})$ corresponding to

$$\boldsymbol{S}_{<>}(p_i) = \langle \boldsymbol{S}_a(p_i^{\alpha_i}), \boldsymbol{S}_b(p_i^{\beta_i}) \rangle$$

will only have index $p_i^{\gamma_i}$ if $A_{p_i}(a) \subseteq A_{p_i}(b)$ or *vice versa*. In general, its index will lie in the range $1 \leq |\boldsymbol{S}_{<>}(p_i)| \leq p_i^{\gamma_i}$, where an index of unity implies $\boldsymbol{S}_{<>}(p_i) = \boldsymbol{L}$. This shows the index of $\boldsymbol{S}_{<>}$ must lie in the range $1 \leq |\boldsymbol{S}_{<>}| \leq (m,n)$ and be a divisor of (m,n).

A parallel argument for $\boldsymbol{S}_{\cap}$ shows its index must be a divisor of mn in the range $mn/(m,n) \leq |\boldsymbol{S}_{\cap}| \leq mn$ and, in fact, that $|\boldsymbol{S}_{<>}||\boldsymbol{S}_{\cap}| = mn$. These relations are illustrated in Figs. 3 and 4.

It is not possible to predict the quotient group structures associated with $\boldsymbol{S}_{<>}$ and $\boldsymbol{S}_{\cap}$ simply from the isomorphism types of the quotient groups of $\boldsymbol{S}_a(m)$ and $\boldsymbol{S}_b(n)$, as they will also depend on the relative orientation in $\boldsymbol{L}$ of the cycles of their Sylow subgroups. Table 1 gives an example of the possibilities relating to two non-isomorphic quotient groups of index 72.

Table 1
Possible quotient group structures that may result from the span and intersection respectively of two index-72 sublattices with individual group structures $C_{24} \otimes C_3$ and $C_{36} \otimes C_2$; $|\boldsymbol{S}_{<>}||\boldsymbol{S}_{\cap}| = 5184$ throughout.

$\lvert S_{<>}\rvert$	$G(S_{<>})$	$G(S_{\cap})$	$\lvert S_{\cap}\rvert$
1	C_1	$C_{72} \otimes C_{12} \otimes C_6$	5184
2	C_2	$C_{72} \otimes C_{12} \otimes C_3$	2592
3	C_3	$C_{72} \otimes C_{12} \otimes C_2$	1728
4	C_4	$C_{72} \otimes C_6 \otimes C_3$	1296
6	C_6	$C_{72} \otimes C_{12}$	864
12	C_{12}	$C_{72} \otimes C_6$	432

3. Algorithms

In practice, a sublattice will commonly be represented by an arbitrary non-singular integral matrix $\boldsymbol{M}$ acting on the vectors of $\boldsymbol{L}$ by premultiplication. From this we may extract the Hermite and Smith normal forms by standard algorithms (Cohen, 1993; Pohst & Zassenhaus, 1989).

The individual sublattices in equation (5) we find by working through the prime divisors of n as shown below for the first prime p_1, for if

$$S(n) = \begin{pmatrix} ap_1^q & d & e \\ 0 & bp_1^r & f \\ 0 & 0 & cp_1^s \end{pmatrix},$$

$(p_1, abc) = 1$, then we have $S(n) = S(p_1^{q+r+s}) \cap S(abc)$ with

$$S(p_1^{q+r+s}) = \begin{pmatrix} p_1^q & d \bmod p_1^q & e \bmod p_1^q \\ 0 & p_1^r & f \bmod p_1^r \\ 0 & 0 & p_1^s \end{pmatrix}$$

and

$$S(abc) = \begin{pmatrix} a & d \bmod a & e \bmod a \\ 0 & b & f \bmod b \\ 0 & 0 & c \end{pmatrix}.$$

The results of the binary operations can be expressed in terms of the sublattices of equations (5) and (9), *i.e.*

$$\boldsymbol{S}_{\cap} = \boldsymbol{S}_a(m) \cap \boldsymbol{S}_b(n) = \bigcap_i [\boldsymbol{S}_a(p_i^{\alpha_i}) \cap \boldsymbol{S}_b(p_i^{\beta_i})]$$

and

$$\boldsymbol{S}_{<>} = \langle \boldsymbol{S}_a(m), \boldsymbol{S}_b(n) \rangle = \bigcap_i \langle \boldsymbol{S}_a(p_i^{\alpha_i}), \boldsymbol{S}_b(p_i^{\beta_i}) \rangle.$$

With this approach, we need only address those primes that divide both m and n, since for an arbitrary prime p

$$\begin{pmatrix} p^0 & 0 & 0 \\ 0 & p^0 & 0 \\ 0 & 0 & p^0 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

$$\begin{pmatrix} p^q & d & e \\ 0 & p^r & f \\ 0 & 0 & p^s \end{pmatrix} \cap \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} p^q & d & e \\ 0 & p^r & f \\ 0 & 0 & p^s \end{pmatrix}$$

and

$$\left\langle \begin{pmatrix} p^q & d & e \\ 0 & p^r & f \\ 0 & 0 & p^s \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \right\rangle = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

For the intersection

$$\begin{pmatrix} p^\alpha & \delta & \varepsilon \\ 0 & p^\beta & \phi \\ 0 & 0 & p^\gamma \end{pmatrix} = \begin{pmatrix} p^A & D & E \\ 0 & p^B & F \\ 0 & 0 & p^C \end{pmatrix} \cap \begin{pmatrix} p^a & d & e \\ 0 & p^b & f \\ 0 & 0 & p^c \end{pmatrix}$$

we have, for the diagonal elements, $\alpha = \max(A, a)$, $\max(b, B) \leq \beta \leq (B + b)$, and $\max(C, c) \leq \gamma \leq (C + c)$, that is, $S_\cap(1, 1)$ is the only non-zero element that can be determined immediately. So we first resolve the upper left submatrix

$$\begin{pmatrix} p^\alpha & \delta \\ 0 & p^\beta \end{pmatrix}$$

by a search through the possible values of β for a solution to

$$p^{\beta-B}D \equiv p^{\beta-b}d \equiv \delta \bmod p^\alpha.$$

The remaining entries derive in a similar way from the simultaneous simplest solutions of congruences on the other two 2×2 submatrices

$$\begin{pmatrix} p^\alpha & \varepsilon \\ 0 & p^\gamma \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} p^\beta & \phi \\ 0 & p^\gamma \end{pmatrix}.$$

In the case of the span

$$\begin{pmatrix} p^\alpha & \delta & \varepsilon \\ 0 & p^\beta & \phi \\ 0 & 0 & p^\gamma \end{pmatrix} = \left\langle \begin{pmatrix} p^A & D & E \\ 0 & p^B & F \\ 0 & 0 & p^C \end{pmatrix}, \begin{pmatrix} p^a & d & e \\ 0 & p^b & f \\ 0 & 0 & p^c \end{pmatrix} \right\rangle,$$

we have for the diagonal elements $1 \leq \alpha \leq \min(A, a)$, $1 \leq \beta \leq \min(B, b)$ and $\gamma = \min(C, c)$.

This time it is the element $S_{<>}(3, 3)$ that can be identified immediately, and we begin by resolving the lower right submatrix

$$\begin{pmatrix} p^\beta & \phi \\ 0 & p^\gamma \end{pmatrix}.$$

Writing for simplicity Γ for $\max(C, c)$, we consider the distribution of values of y for which the plane (x, y, p^Γ) includes points of either sublattice. This leads to the values of β and ϕ being given by the largest value of β for which a congruence $\phi \equiv (p^{\Gamma-C}F - p^{\Gamma-c}f) \bmod p^\beta$ exists. Similarly to the previous case, the completion of the process depends on the simultaneous resolution of the two remaining submatrices.

I wish to thank one of the anonymous referees for suggesting significant improvements to this article.

References

Bärnighausen, H. (1980). *MATCH – Commun. Math. Chem.* **9**, 139–175.

Billiet, Y. & Rolley-Le Coz, M. (1980). *Acta Cryst.* A**36**, 242–248.

Cohen, H. (1993). *Computational Algebraic Number Theory.* Berlin: Springer-Verlag.

Conway, J. H. & Sloane, N. J. A. (1988). *Sphere Packings, Lattices and Groups.* New York: Springer-Verlag.

Gruber, B. (1997). *Acta Cryst.* A**53**, 807–808.

Harker, D. (1978). *Proc. Natl Acad. Sci. USA*, **75**, 5264–5276.

Lang, S. (2002). *Algebra*, 3rd ed. Berlin: Springer-Verlag.

Pohst, M. & Zassenhaus, H. (1989). *Arithmetic Algebraic Number Theory*. Cambridge University Press.

Polya, G. & Read, R. C. (1987). *Combinatorial Enumeration of Groups, Graphs and Chemical Compounds.* New York: Springer-Verlag.

Rutherford, J. S. (1992). *Acta Cryst.* A**48**, 500–508.

Rutherford, J. S. (1993). *Acta Cryst.* A**49**, 293–300.

Rutherford, J. S. (1995). *Acta Cryst.* A**51**, 672–679.

Rutherford, J. S. (2003). *Cryst. Eng.* **6**, 225–234.

Stokes, H. T. & Hatch, D. M. (2002). *Phys. Rev. B*, **65**, 144114.

Wondratschek, H. & Aroyo, M. I. (2001). *Acta Cryst.* A**57**, 311–320.