5. Concluding remarks

The theory of time-dependent X-ray Bragg diffraction by a crystal is developed allowing for the effects of the partial time and space coherence of the incident beam. It is found that, for the case where the input wave is plane (or is the incoherent superposition of plane waves) and the amplitude is a δ function in time (the ultrashort time pulse approximation), the instantaneous crystal reflectivity is a smooth temporal function. Furthermore, in the limit where the observation time t is much longer than the characteristic value t_o [$t_o = \Lambda/2\pi c$ and $t_o = (\mu_o c)^{-1}$, respectively, for the dynamical and kinematical Bragg diffraction], the crystal reflectivity tends to the value for the integrated Bragg reflectivity calculated by CDKT. If the input X-ray pulse profile is a pseudo δ function in both time and space, the temporal crystal response has a functional dependence identical with that of the spatial distribution of the diffracted intensity under the conventional Bragg diffraction of the X-ray beam with the lateral width $t_o c$.

In the general case, where the input X-ray pulse is partially coherent in time and space, calculations of practical interest can be carried out with the formulae (20)–(22). The important conclusion following from this study is that the temporal crystal response is determined by the characteristic length when the input duration length is much smaller than the latter. So, taking into account that for the X-rays the typical values are $\Lambda/2\pi \simeq 3\,\mu$m and $\mu_o \simeq 60\,\mu$m, $t_o \simeq 10$ fs and $t_o \simeq 200$ fs for the dynamical and kinematical Bragg diffraction, respectively. The last value of t_o for the kinematical Bragg diffraction is comparable with the time duration of ultrashort X-ray pulse sources by the interaction of intense laser pulses with solid targets (Uschmann *et al.*, 1995). The present calculations will have potential applications in time-dependent X-ray optics when X-ray pulse sources with a comparable time duration come to be used in practice.

Also notice that thermal neutrons may also be used in place of X-rays and offer another opportunity to observe the time-delay effect since in this case the value of the characteristic time is increased.

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The Enumeration and Symmetry-Significant Properties of Derivative Lattices. III. Periodic Colourings of a Lattice

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Abstract

In the triclinic case, structures that can be described in terms of arrangements of a set number of possible subunits occupying the unit cells of an underlying lattice may be enumerated by their derivative lattice index n and stoichiometry, *e.g.* $X_m Y_{(n-m)}$ for two types of subunits. This process involves counting the number, $H(n, m)$, of such patterns possible on the frame of the colour lattice group, followed by the elimination of any patterns that belong to a derivative lattice of lower index. The resulting numbers, $K(n, m)$, then have the property

$$K(n, m) \leq (1/n)\binom{n}{m} \leq H(n, m)$$

where $\binom{n}{m}$ is the binomial coefficient. These expressions are equalities if n and m are mutually prime. $H(n, m)$ and

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$K(n, m)$ are tabulated for all colour lattice groups $n \leq 20$ and all corresponding values of m. The method may be extended to a larger number of subunit types by a simple change to the figure-generating function.

Introduction

This series of papers on the enumeration of derivative lattices (Rutherford, 1992, 1993), together with some parallel work on graph theory approaches to the bond-valence distribution in solids (Rutherford, 1990, 1991), represents an attempt to explore the potential that mathematical chemistry, *i.e.* the application of graph theory and combinatorics to chemistry, holds for the enrichment of crystallography.

One important concept of combinatorics is the generating function, where the number of distinct objects with a given property is simply the coefficient of one term in the expansion of that function. The application of power-series generating functions to isomer-counting problems in chemistry derives mainly from Polya (1937). Generating functions have the advantage, besides elegance and compactness, of their usefulness in deriving statistical information on, and asymptotic estimates of, the number of isomers (or other geometric objects) involved in the enumeration. In order to construct an equivalent theory of derivative lattices, we shall have to consider two types of generating functions, the Polya type and the Dirichlet type (Hardy & Wright, 1979).

Derivative lattices (Billiet & Bertaut, 1983) arise in practice both as real lattices (commensurate superlattices) and as reciprocal lattices, in the consideration of phase-determining techniques, and, in particular, as problems of rational dependence between large structure factors. In fact, it was originally to gain statistical information for a test of such rational dependence that Dirichlet generating functions were introduced to crystallography (Rutherford, 1992). The generating functions were derived to provide, for each Patterson symmetry of the basic lattice, the number of derivative lattices of equal index with the same point-group symmetry. A second paper (Rutherford, 1993) extended this approach of using Dirichlet functions to an enumeration of derivative lattices, now in the general case only, but in terms of their classification by colour lattice group (Harker, 1978) rather than just index. The present paper is intended to show that it leads to a much improved method of attack on those structural enumerations recognized by McLarnan & Moore (1981) as lattice-colouring problems for which Polya's method may be applied.

Polya enumeration in crystallography

One aspect of mathematical chemistry that has been extensively investigated is the application of Polya's theorem (Polya, 1937; Polya & Read, 1987), *i.e.* that the total pattern inventory is represented by the coefficients in the expansion of the cycle sum:

$$S = \sum_{d|n} F(d) a_d^{n/d},$$

where the sum is over the divisors d of n and F_d is the cycle sum coefficient, *i.e.* effectively the number of locations in the frame, on which the patterns are arranged, which fall on a cycle of minimum length d with respect to the frame symmetry group. Polya & Read (1987) give an extensive bibliography of results for molecules and similar finite systems and Fujita (1990) gives numerous more recent references. However, its application to periodic systems such as crystals and crystal surfaces has received scant attention. McLarnan & Moore (1981) reviewed the work done at that time in the area of crystal structure in general; even here, however, it is clear that the major interest has been in finite molecules and clusters. The extension of the approach to what McLarnan & Moore (1981) describe as colouring problems has largely been ignored and, in fact, most of the relevant work to date has been done by these authors themselves (Moore & Araki, 1976; McLarnan, 1978, 1981). As McLarnan & Moore (1981) point out, there is a basic difficulty in enumerating the arrangements that may occur for this type of problem, in that Polya's theorem must normally be based on a specific algebraic structure, the frame group, which is the symmetry group of the molecular graph or coordination polyhedron in finite examples, but which corresponds to a specific unit cell in the crystallographic case. The unit cells that arise in turn represent derivative lattices of index n of some underlying lattice, on which the possible distinct structures comprise arrangements of N colours representing structure elements. These colours may be arranged, with a particular colour occupying a lattice point for each structural element that may occur in that site (basis lattice unit cell), according to their full permutation group ($N \leq n$). This is the situation, rather than the more restricted case of the colour symmetry group for which $n = N$, that is relevant to most counting problems involving structural derivative lattices.

Essentially, the reason for McLarnan & Moore's (1981) difficulties was that at the time each derivative lattice had to be considered separately, and there was no general method of enumeration of either the derivative lattices involved or their individual colour lattice groups. In fact, on the question of the number of distinct derivative lattices of index n for a given basic lattice, the required relationships were established in general by Bertaut & Billiet (1979) and the triclinic case was studied in detail by Billiet & Rolley-Le Coz (1980). The latter expressed their results in terms of restrictions on the possible integral elements of standard triangular transformation matrices of determinant n. This led Rutherford (1992) to introduce Dirichlet generating functions into crystallography to provide a more convenient tool in the enumeration of such derivative lattices.

Although the coloured symmetry groups have been the subject of extensive research for a number of years, the specific result relevant to our second question, namely the possible forms taken by the translational subgroups in N colours, was only resolved by Harker in 1978. He recognized that in three dimensions they were the Abelian groups of stable form $C_{fhg} \times C_{fg} \times C_f$,* of order $N = f^3g^2h, f, g$ and h being positive integers. Soon after, the number of such groups was derived by Kucab (1981). However, it was only recently that the details of the distribution of the non-isomorphous colour lattice groups among the derivative lattices of equal index were worked out (Rutherford, 1993).

It now seemed appropriate to examine the possibility that this crystallographic colouring problem might be freed from the limitations imposed by dealing with each unit cell individually. It is the purpose of this paper to show that this is indeed the case, and to indicate the further problems that must be overcome in its solution. This exposition will assume two colours only, *i.e.* it will apply the figure-generating function

$$a_d = (x^d + y^d),$$

where the coefficient of the term in $x^b y^{n-b}$ gives the number of patterns with b occurences of the first colour. The extension of the method to any number of colours $N \leq n$ involves only a straightforward change to the figure-generating function.

Method

The method followed consists of four steps, namely:

(1) The enumeration of the derivative lattices of a given lattice by index (number of points of the basic lattice in each unit cell of the derivative lattice) using arithmetic functions. It is possible to include crystal symmetry constraints in this enumeration, but for simplicity this paper will deal only with the asymmetric case. The details of this procedure have already been published (Rutherford, 1992).

(2) The identification of the various algebraic structures (colour lattice groups) that may occur for derivative lattices of a particular index (Harker, 1978) and the partition of the total number of derivative lattices for that index, as found in the previous section, by structure (Rutherford, 1993).

(3) The application of Polya's theorem to provide the total number of patterns for each algebraic structure present, categorized according to the number of points of each colour making up the derivative lattice.

(4) The elimination from the count for that index of patterns that correspond to a derivative lattice of lower index, that index being a factor of the one under consideration. Such cases will have been already counted under that lower index.

As an example of this, we may consider the arrangement of eight figures, four black and four white, on the frame $C_4 \times C_2$. We then find Polya's formula predicts

$$\begin{aligned} H(n,m) &= (1,n) \sum_{d|n,m} F_d \begin{bmatrix} n/d \\ m/d \end{bmatrix} \\ &= \tfrac{1}{8} \sum_{d|8,4} F_d \begin{bmatrix} 8/d \\ 4/d \end{bmatrix} \\ &= \tfrac{1}{8}(1 \times 70 + 3 \times 6 + 4 \times 2) \\ &= 12. \end{aligned}$$

Here $d|n, m$ implies d is a divisor of both n and m, and $\begin{bmatrix} n \\ m \end{bmatrix}$ is the binomial coefficient. These 12 patterns are illustrated in Fig. 1. However, of these 12, five (a to e in Fig. 1) produce derivative lattices of small true index when infinitely repeated in two or more dimensions, while only the remaining seven produce true index eight derivative lattices.

As in the previous papers, the method will be illustrated by presenting first the relatively simple one-dimensional case and extending the arguments to two and finally three dimensions.

Multiplicative number theory

The reader is referred to the previous papers (Rutherford, 1992, 1993) and references therein, particularly Hardy & Wright (1979), for a detailed discussion of the relevant

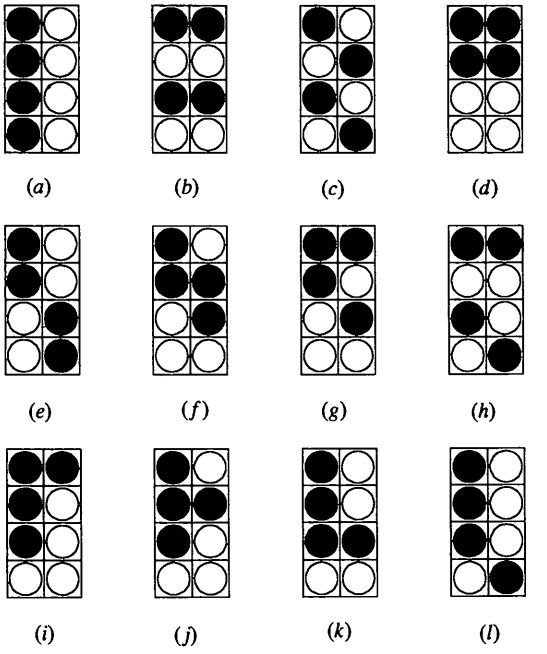

Fig. 1. Patterns that may be arranged on $C_4 \times C_2$. The corresponding derivative lattice indices are: (*a*)–(*c*) 2; (*d*)–(*e*) 4; (*f*)–(*l*) 8.

* Strictly speaking, the colour lattice groups are infinite Abelian groups and these finite groups are their torsion subgroups; however, we shall continue to refer to the finite groups as the colour lattice groups since it is their properties that are all important to the analysis.

multiplicative arithmetic functions and Dirichlet series. Briefly, we shall be interested in Dirichlet series of the type

$$F(s) = \sum_{n=1}^{\infty} \alpha_n n^{-s},$$

where $F(s)$ is the generating function of some α_n, the corresponding arithmetic function. Here α_n simply enumerates some property associated with the natural number n, and in such cases the variable s has no real significance. The series of interest are 'multiplicative' in the number-theory sense, *i.e.* α_n are multiplicative over the primes. In other words,

$$\alpha_m \alpha_n = \alpha_{mn},$$

provided m and n have no common factor. We shall use this multiplicative property in constructing the required arithmetic functions.

We shall, however, require two results not included previously. The first is the Möbius inversion formula, *i.e.*

$$F(n) = \sum_{d|n} G(d),$$

implies

$$G(n) = \sum_{d|n} \mu(d) F(d),$$

where F and G are multiplicative arithmetic functions, $d|n$ again indicates d is a divisor of n, and μ is the Möbius function $\mu(n)$, defined as: $\mu(a) = 1$ if $a = 1$; $\mu(a) = (-1)^r$ if a is the product of r distinct prime factors, *i.e.* if a is square-free (contains no repeated factors); $\mu(a) = 0$ otherwise, *i.e.* if a is divisible by the square of a prime.

The second requirement is to introduce the Euler totient function, $\varphi(n)$, which is the number of positive integers less than and mutally prime to n. For example, $\varphi(5) = 4$, the number of elements of $\{1,2,3,4\}$, and $\varphi(6) = 2$, for $\{1,5\}$. $\varphi(1)$ is defined as unity. $\varphi(n)$ is multiplicative in the primes; for example, the relevant set for $n = 15$ is $\{1,2,4,7,8,11,13,14\}$, and so

$$\varphi(15) = 8 = 2 \times 4 = \varphi(3)\varphi(5).$$

Since $\varphi(n)$ is a multiplicative arithmetic function, there ought to be a corresponding Dirichlet-series-generating function, which indeed proves to be:

$$\zeta(s-1)/\zeta(s) = \sum_{n=1}^{\infty} \varphi(n) n^{-s},$$

where $\zeta(s)$ is the Riemann ζ function. However, if we use the general formula for a product of Dirichlet functions, namely

$$F(s)G(s) = \sum_{n=1}^{\infty} \left\{ \sum_{d|n} f(n/d)g(d) \right\} n^{-s},$$

we can deduce that $\zeta^{-1}(s)\zeta(s-1)$ generates

$$\sum_{d|n} \mu(n/d)d$$

and thus establish the identity

$$\varphi(n) = \sum_{d|n} \mu(n/d)d.$$

For example,

$$\begin{aligned}\varphi(12) &= \mu(12) \times 1 + \mu(6) \times 2 + \mu(4) \times 3 + \mu(3) \times 4 \\ &\quad + \mu(2) \times 6 + \mu(1) \times 12 \\ &= 0 \times 1 + 1 \times 2 + 0 \times 3 + (-1) \times 4 \\ &\quad + (-1) \times 6 + 1 \times 12 \\ &= 4.\end{aligned}$$

One-dimensional case

The number of one-dimensional lattices of index n is one only for each n and is therefore enumerated by

$$\zeta(s) = \sum_{n=1}^{\infty} 1 \times n^{-s}.$$

Since there is only one lattice for each n, there can be only one structure, which is that of the cyclic group C_n. This is consistent with the number of such groups also being enumerated by

$$\zeta(s) = \sum_{n=1}^{\infty} 1 \times n^{-s}.$$

Polya's theorem is simple to apply in the case of C_n for a specific n; however, what we seek is an expression for the cycle sum for such a cyclic group for general n. The cycle sum takes the form

$$S = \sum_{d|n} F(d) a_d^{n/d},$$

where the sum is over the divisors d of n, there being only one cycle C_d for each divisor. Now it is known that we can write $F(d)$ as the totient function $\varphi(d)$ but, equivalently, we may use the fact that each of the d elements of a cycle C_d must either count in the sum $F(d)$ for the C_d or in one of its factors, *e.g.* $F(b)$; $b|d$. Also, all the cycles present can be broken down in terms of the separate prime factors involved, *i.e.* the structure is multiplicative in the sense $C_{mn} = C_m \times C_n$, provided m and n are mutually prime.

This tells us that we seek for the cycle-sum coefficient $F(d)$ a multiplicative function which has the property

$$d = \sum_{b|d} F(b).$$

The technique of Möbius inversion then gives

$$F(d) = \sum_{b|d} \mu(d/b) b$$

for the cycle-sum coefficient. This means the cycle sum becomes

$$S = \sum_{d|n} \left[\sum_{b|d} \mu(d/b)b \right] a_d^{n/d}$$

or, alternatively,

$$S = \sum_{d|n} \varphi(d) a_d^{n/d}.$$

Now, for an arrangemet involving m points of one colour and $(n-m)$ of the other, we simply substitute $(x^d + y^d)$ for each a_d and combine the coefficients of $x^m y^{(n-m)}$ in the resulting binomial expansion, to give the total pattern inventory

$$(1/n) \sum_{d|n,m} \varphi(d) \begin{bmatrix} n/d \\ m/d \end{bmatrix}.$$

There are two important things to be noticed about this formula. The first is that only those terms where $d|m$, $(n-m)$, contribute to the total number of arrangements for given m. The second is the factor $1/n$, which arises because the cycle-sum approach generates each pattern n times identically except for a shift of origin. In order to extend this approach to three colours, we would apply the figure-generating function

$$a_d = (x^d + y^d + z^d)$$

and so on.

This completes the third step of the method for this case. The need for a fourth step arises from the infinite (or quasi-infinite) repetitive character of the crystal lattice. We can illustrate this distinction, for what is otherwise an identical cyclic frame group C_n, by the common example of coloured beads threaded on a necklace. There, although the finite sequences $(bwbw)$ and $(bwbwbw)$ have the same stoichiometry, they represent distinct necklaces of frame groups C_4 and C_6, respectively, while the sequences $(bwbw)_\infty$ and $(bwbwbw)_\infty$ from an identical linear chain, for which the true representation is $(bw)_\infty$, of frame group C_2. Thus, the pattern inventories derived above will contain elements of true index d, $d|n, m$, for at least some of the possible values of d.

If we write the number of elements of the total pattern inventory as $H(n, m)$ and that of the patterns of true index n as $K(n, m)$, we can then use the identity

$$H(n, m) = \sum_{d|n,m} K(n/d, m/d)$$

to describe the fourth step as a recursive process:

$$K(n, m) = H(n, m) - \sum_{d(>1)|n,m} K(n/d, m/d).$$

For the one-dimensional case, we have

$$H(n, m) = (1/n) \sum_{d|n} \varphi(d) \begin{bmatrix} n/d \\ m/d \end{bmatrix};$$

however, in this particular case there are no complications in applying the inclusion/exclusion principle to the patterns that occur, which then allows us to use the Möbius inversion to carry out the summation involved in calculating $K(n, m)$;

$$K(n, m) = \sum_{d|n,m} \mu(d) H(n/m, m/d)$$

$$= (1/n) \sum_{d|n,m} \mu(d) d \left\{ \sum_{bd|n,m} \varphi(b) \begin{bmatrix} n/bd \\ m/bd \end{bmatrix} \right\}.$$

As an application of this formula, consider six black and six white figures arranged on the periodic frame C_{12}.

$$K(12, 6) - (1/12) \sum_{d|12,6} \mu(d) d \left\{ \sum_{bd|12,6} \varphi(b) \begin{bmatrix} 12/bd \\ 6/bd \end{bmatrix} \right\}.$$

Possible values of d and b, respectively, are:

(1,1); (1,2); (1,3); (1,6); (2,1); (2,3); (3,1); (3,2); (6,1).

The sum therefore becomes

$$(1/12)\left(1 \times 1\left\{\begin{bmatrix} 12 \\ 6 \end{bmatrix} + \begin{bmatrix} 6 \\ 3 \end{bmatrix} + 2\begin{bmatrix} 4 \\ 2 \end{bmatrix} + 2\begin{bmatrix} 2 \\ 1 \end{bmatrix}\right\}\right.$$
$$+ (-1) \times 2\left\{\begin{bmatrix} 6 \\ 3 \end{bmatrix} + 2\begin{bmatrix} 2 \\ 1 \end{bmatrix}\right\} + (-1) \times 3\left\{\begin{bmatrix} 4 \\ 2 \end{bmatrix} + \begin{bmatrix} 2 \\ 1 \end{bmatrix}\right\}$$
$$\left. + 1 \times 6\left\{\begin{bmatrix} 2 \\ 1 \end{bmatrix}\right\}\right) = 75.$$

In the case of a finite figure, the corresponding cycle sum would be simply the first grouped term:

$$(1/12)\left\{\begin{bmatrix} 12 \\ 6 \end{bmatrix} + \begin{bmatrix} 6 \\ 3 \end{bmatrix} + 2\begin{bmatrix} 4 \\ 2 \end{bmatrix} + 2\begin{bmatrix} 2 \\ 1 \end{bmatrix}\right\} = 80.$$

This shows that, for this example, five patterns of the 80 that occur for a finite frame group have a smaller true index when applied to a lattice. These comprise one of index 2, one of index 4 and three of index 6.

Two-dimensional case

Here, the function that enumerates the lattices of index n is

$$\zeta(s)\zeta(s-1) = \sum_{n=1}^{\infty} \sigma_1(n) n^{-s},$$

where $\sigma_1(n)$ is the sum of the divisors of n. The number of distinct algebraic structures in two dimensions is given by the expansion of $\zeta(s)\zeta(2s)$. Now we have to identify how the overall $\sigma_1(n)$ lattices are distributed over the possible structures. This breakdown depends on a new arithmetic function $q_2(n)$ which is generated by $\zeta(s) \times \zeta^{-1}(2s)$, and in fact the number of lattices with colour lattice group $C_{fg} \times C_f$ can be shown, by suitable manipulation of the generating functions, to be

$$\sum_{d|g} (g/d) q_2(d).$$

Now, most of these lattices correspond to structures with $f = 1$, *i.e.* they have identical structures to the one-dimensional case. However, in order to take into account the truly two-dimensional structures, we must now examine in detail the structure of the Abelian group $C_{fg} \times C_f$, of order $n = f^2 g$. For such groups, the number of subgroups of the form $C_{ab|fg} \times C_{a|f}$ is multiplicative, and therefore it is sufficient to determine the relevant structure for each prime factor of n. Let us call this structure $C_{p^\beta} \times C_{p^\alpha}$ and designate subgroups of this $C_{p^\delta} \times C_{p^\gamma}$, where $\beta \geq \alpha$, $\beta \geq \delta$, $\delta \geq \gamma$ and $\alpha \geq \gamma$. Then, if $\delta > \alpha$, the number of such subgroups, $N(C_{p^\delta} \times C_{p^\gamma})$, is simply $p^{\alpha-\gamma}$. However, if $\delta \leq \alpha$, such subgroups are also subgroups of the single subgroup of structure $C_{p^\alpha} \times C_{p^\alpha}$. This allows us, for cases where $1 \leq (\gamma + \delta) \leq \alpha$, to treat this problem as equivalent to the number of lattices of that structure as dealt with above, namely

$$\begin{aligned} N(C_{p^\delta} \times C_{p^\gamma}) &= \sum_{d|p^{\gamma+\delta}} q_2(d)[p^{\gamma+\delta}/d] \\ &= \sum_{i=0}^{\gamma+\delta} q_2(p^i) p^{\gamma+\delta-i} \\ &= (p+1)p^{\gamma+\delta-1}, \end{aligned}$$

since $q_2(p^i)$ is non-zero only for $i = 0$ or 1. Also, for $\delta \leq a$ and $\alpha \leq (\gamma + \delta) \leq 2\alpha$, the number of subgroups is equal to that of quotient groups $C_{p^{(\alpha-\gamma)}} \times C_{p^{(\alpha-\delta)}}$ of order $p^{(2n-\gamma-\delta)}$, which has already been determined, since now $0 \leq (2\alpha - \gamma - \delta) \leq \alpha$.

To summarize:

$$\begin{aligned} &N(C_{p^\delta} \times C_{p^\gamma}) = (p+1)p^{\gamma+\delta-1} && \text{if } \delta \leq \alpha,\ 1 \leq (\gamma+\delta) \leq \alpha \\ &N(C_{p^\delta} \times C_{p^\gamma}) = (p+1)p^{2\alpha-(\gamma+\delta)-1} && \text{if } \delta \leq \alpha,\ \alpha \leq (\gamma+\delta) \leq 2\alpha \\ &N(C_{p^\delta} \times C_{p^\gamma}) = 1 && \text{if } \delta = \gamma = \alpha \\ &N(C_{p^\delta} \times C_{p^\gamma}) = p^{\alpha-\gamma} && \text{if } \delta > \alpha. \end{aligned}$$

The cyclic subgroups that we require to count for the cycle index are particular cases of the general subgroups above, for which $\gamma = 0$. Thus, they may be counted as follows (making the substitution $\gamma = 0$ in the formulae above):

$$\begin{aligned} &(p+1)p^{\delta-1} && \text{if } \delta \leq \alpha \\ &p^\alpha && \text{if } \delta > \alpha. \end{aligned}$$

This in turn yields for the number of cyclic subgroups of order $d|n$:

$$\prod_{p_i^{\delta_i} \| f} p_i^{\alpha_i} \prod_{p_j^{\delta_j} | f} (p_j + 1) p_j^{\delta_j - 1},$$

where

$$d = \prod_{p_i | d} p_i^{\delta_i}.$$

Now,

$$F_d = \varphi(d) \left\{ \prod_{p_i^{\delta_i} \| f} p_i^{\alpha_i} \prod_{p_j^{\delta_j} | f} (p_j + 1) p_j^{\delta_j - 1} \right\}.$$

Polya's theorem may now be applied; however, the final step of identifying the patterns of lower true index is now more difficult, since the Möbius function method no longer applies and we must carry out the recursion over the subgroups G_d of the colour lattice group G:

$$K(n, m) = H(n, m) - \sum_{G_d | G} K(n/d, m/d) \qquad d(> 1) | n, m.$$

Here, d is the index of the subgroup in G; its order, and the index of the corresponding lattice, is (n/d).

For example, for the group $C_6 \times C_2$, $n = 12$ and $m = 6$, we have:

$$K(12, 6) = H(12, 6) - \sum_d K(12/d, 6/d)$$

$$G_d(d > 1) | C_6 \times C_2.$$

Possible values of d are 2, 3 and 6 and therefore G_d can only be C_6, $C_2 \times C_2$ or C_2, there being no C_4 subgroup.

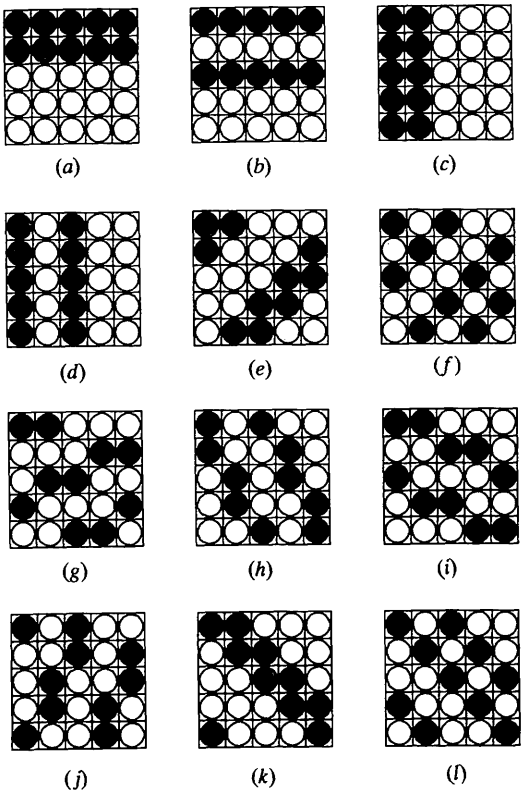

Fig. 2. The 12 patterns of index 5 and stoichiometry A_3B_2. The corresponding unit cells have basis vectors: (*a*)–(*b*) $5a, b$; (*c*)–(*d*) $a, 5b$; (*e*)–(*f*) $a - b, a + 4b$; (*g*)–(*h*) $a - 2b, a + 3b$; (*i*)–(*j*) $a - 3b, a + 2b$; (*k*)–(*l*) $a - 4b, a + b$; where a is vertical and b horizontal.

Table 1. *$K(n, m)$ and $H(n, m)$ for all colour lattice groups $C_{fgh} \times C_{fg} \times C_f$ of order $n \leq 20$ and relevant m; $H(n, m)$ is in parentheses below where different from $K(n, m)$*

		m									
n	*h,g,f*	1	2	3	4	5	6	7	8	9	10
2		1									
3		1									
4	4,1,1	1	1								
			(2)								
	1,2,1	1	0								
			(3)								
5		1	2								
6		1	2	3							
			(3)	(4)							
7		1	3	5							
8	8,1,1	1	3	7	8						
			(4)		(10)						
	2,2,1	1	2	7	7						
			(5)		(12)						
	1,1,2	1	0	7	7						
			(7)		(14)						
9	9,1,1	1	4	9	14						
				(10)							
	1,3,1	1	4	8	14						
				(12)							
10		1	4	12	20	25					
			(5)		(22)	(26)					
11		1	5	15	30	42					
12	12,1,1	1	5	18	40	66	75				
			(6)	(19)	(43)		(80)				
	3,2,1	1	4	18	38	66	72				
			(7)	(19)	(45)		(84)				
13		1	6	22	55	99	132				
14		1	6	26	70	143	212	245			
			(7)		(73)		(217)	(246)			
15		1	7	30	91	200	333	429			
				(31)		(201)	(335)				
16	16,1,1	1	7	35	112	273	497	715	800		
			(8)		(116)		(504)		(810)		
	4,2,1	1	6	35	109	273	490	715	792		
			(9)		(120)		(511)		(820)		
	1,4,1	1	6	35	109	273	490	715	792		
			(9)		(122)		(511)		(822)		
	2,1,2	1	4	35	105	273	476	715	778		
			(11)		(128)		(525)		(838)		
17		1	8	40	140	364	728	1144	1430		
18	18,1,1	1	8	45	168	476	1026	1768	2424	2700	
			(9)	(46)	(172)		(1038)		(2438)	(2704)	
	2,3,1	1	8	44	168	476	1024	1768	2424	2697	
			(9)	(48)	(172)		(1044)		(2438)	(2710)	
19		1	9	51	204	612	1428	2652	3978	4862	
20	20,1,1	1	9	57	240	775	1932	3876	6288	8398	9225
			(10)		(245)	(776)	(1944)		(6310)		(9252)
	5,2,1	1	8	57	236	775	1920	3876	6268	8398	9200
			(11)		(249)	(776)	(1956)		(6330)		(9278)

The number of isomorphic subgroups of each of these types are:

C_6	3
$C_2 \times C_2$	1
C_2	3

and thus the evaluation becomes

$$K(12, 6) = 84 - 3 \times 3 - 1 \times 0 - 3 \times 1 = 72.$$

This time there is a total of 84 patterns for a finite frame, but 12 of the these prove to have a smaller true index when applied to the lattice.

Three-dimensional case

The three-dimensional case involves colour lattice groups of the form $C_{fgh} \times C_{fg} \times C_f$. The number of lattices and their breakdown by colour lattice group is determined by*

$$g^2 \sum_{j=1}^{d_3(n/f^3g^2)} q_3(c_{1j}) q_2(c_{2j})\, c_{2j}\, c_{3j}^2,$$

where $d_3(n/f^3g^2)$ is the number of ways of expressing h as a product of three factors, any number of which may

* This formula was misprinted in the previous paper.

be unity, *i.e.*

$$h = n/f^3g^2 = c_{1j}c_{2j}c_{3j},$$

and q_3 is the characteristic function of the cube-free integers, *i.e.* $q_3(n) = 0$ if n is divisible by a cube and $q_3(n) = 1$ otherwise.

Only a small fraction of these lattices have truly three-dimensional structures with $f > 1$ (Rutherford, 1993), and since the general formulae for the numbers of subgroups are complex, these cases were considered individually.

Concluding remarks

After applying Polya's theorem, and removing by recursion the patterns of lower true index, we find $K(n, m)$. Table 1 contains the relevant results for indices up to 20. These may be combined with the number of lattices belonging to each colour lattice group, given in Tables 1 and 2 of Rutherford (1993), to give the total number of patterns; for example, for $n = 5$ and $m = 2$ in two dimensions, we have

$$2\sigma_1(5) = 2 \times 6 = 12$$

possible patterns. These are shown in Fig. 2.

A more complex example in two dimensions is $n = 18$, $m = 6$. Here, there are 36 lattices belonging to colour lattice group C_{18} and 3 to $C_6 \times C_3$. For the former and $m = 6$, the total number of patterns is 1026, the latter 1024. This gives as the total number:

$$(36 \times 1026) + (3 \times 1024) = 40\,008.$$

The number of patterns in three dimensions is considerably larger still; for example, for $n = 16$, $m = 8$, we have

$$(448 \times 800) + (168 \times 792) + (28 \times 792) + (7 \times 778) = 519\,078.$$

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The Validity of Approximations Made in Differential Anomalous X-ray Scattering

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Abstract

Approximations of weighting-factor functions are used when determining coordination numbers from differential anomalous scattering (DAS) experiments. The accuracy of two single-value approximations for the weighting functions are tested using non-interacting hard-sphere models of systems that have been studied previously with DAS. The first approximation is an average of the weighting-factor function over the experimental wave-vector range. The second is the weighting-function value at the wave vector that is related to a peak position in the corresponding differential radial distribution function (dRDF). It was found that the first approximation introduced up to 10% error into calculated coordination numbers. The second weighting-factor approximation introduced minimal error into the coordination-number calculations and is simple to use.

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