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A New Method of Generating Plane Groups of Simple and Multiple Antisymmetry

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Abstract

A new method of generating groups of simple and multiple antisymmetry of M^m type, based on presentations of groups of symmetry and on a newly defined term of antisymmetric characteristics, is suggested and applied to generate plane groups of simple and multiple antisymmetry of M^m type from 17 plane groups of symmetry.

The terms simple and multiple antisymmetry have been used in this study in accordance with the definitions given by Shubnikov, Belov, Neronova, Smirnova, Tarkhova & Belova (1964), Zamorzaev (1963, 1976), Shubnikov & Koptsik (1972) and Zamorzaev & Palistrant (1980). The G' group of simple antisymmetry is the combination of the discrete G group of symmetry and the transformation of antiidentity of the first kind e_1 which satisfy the relations (α) $i=j=1$, *i.e.* $e_i^2=E$, $e_1S_q=S_qe_1$, $q\in\{1,2,\ldots,p\}$, and the G' group of multiple antisymmetry is the combination of G with l antiidentities $e_1, e_2, \ldots, e_l$ and with its products, which satisfy relations (α). The effect of antiidentities $e_1, e_2, \ldots, e_l$ can be interpreted by the system of (geometrical or non-geometrical) mutually commutative and independent alternating two-phase changes [(+, −), (black, white), ...], commutative with the generators S_q, $q\in\{1,2,\ldots,p\}$ of the G group. The plane crystallographic groups of simple and multiple antisymmetry have been discussed separately, in detail, by Mackay (1957), Belov & Belova (1957), Zamorzaev & Palistrant (1960, 1961), Palistrant (1965), Loeb (1971) and Zamorzaev (1976).

The derivation of groups of simple and multiple antisymmetry of M^m type generated from seventeen two-dimensional plane crystallographic groups will be achieved in this study by the application of the method suggested by Jablan (1984) and is founded on the following theoretical suppostions:

Let the discrete symmetry group G with a set of generators $\{S_1, S_2, \ldots, S_p\}$ be represented by (Coxeter & Moser 1972)

$$g_n(S_1,\ldots,S_p)=E,\ n=1,2,\ldots,s,$$

and let $e_1, e_2, \ldots, e_l$ be antiidentities of the first, second, ..., lth kind, which satisfy the relations

$$e_ie_j=e_je_i,\qquad e_i^2=E\qquad e_iS_q=S_qe_i,$$
$$i,j\in\{1,2,\ldots,l\},\ q\in\{1,2,\ldots,p\}.\qquad(1)$$

The groups of simple and multiple antisymmetry are derived by applying the general method of Shubnikov–Zamorzaev (Zamorzaev, 1976), *i.e.* by substituting the generators of the G group with antigenerators of one or several independent kinds of antisymmetry. In accordance with the theorem on dividing all groups of simple and multiple antisymmetry into groups of $C^k(1\le k\le l)$, C^kM^m $(1\le k, m;\ k+m\le l)$ and M^m $(1\le m\le l)$ types (Zamorzaev, 1963, 1976) and with the possibility of deriving the groups of the C^k and C^kM^m types directly from the generating group G and from the groups of M^m type, respectively, the only non-trivial problem appears to be that of deriving the groups of M^m type.

The derivation of the groups of M^m type is founded on the following theorems:

Theorem 1: (The existential criterion for groups of M^m type): The group of simple or multiple antisymmetry G' will be of the M^m type (a) if all relations given within the presentation of the group G remain satisfied after the generators have been substituted by antigenerators and (b) if the antisymmetry of an arbitrary kind can be derived within the antisymmetry group G' as an independent antisymmetrical transformation.

Definition: Let all products of generators of group G, within which all generators participate once at the most, be formed and then separate the subsets of transformations that are equivalent with respect to symmetry. The resulting system is called the antisymmetric characteristic of group G.

Theorem 2: Two groups of simple or multiple antisymmetry G_1' and G_2' of the M^m type for m fixed, with common generating group G, are equal if and only if they possess equal antisymmetric characteristics.

Theorem 3: Groups of M^1 type are derived from the group of symmetry G. All groups of M^m type for

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$p1$	$\{X, Y\}: \{X, Y, XY\}$	For $m = 1$ it is obligatory to substitute two generating translations with antitranslations and for $m = 2$ to substitute all the translations with antitranslations of different kinds.
	$\{X, Y, Z\}: \{X, Y, Z\}$	
$p2$	$\{X, Y, T\}: \{T, TX, TY, TXY\}$	When generating groups of the M^m type, it is possible to make combinations of the antiidentities e_1, e_2, e_3 in which they appear twice or four times, see theorem 1(b).
	$\{T_1, T_2, T_3\}: \{T_1, T_2, T_3, T_1T_2T_3\}$	
	$\{T_1, T_2, T_3, T_4\}: \{T_1, T_2, T_3, T_4\}$	
pm	$\{X, Y, R\}: \{Y\}\{R, RX\}$	
	$\{Y, R, R'\}: \{Y\}\{R, R'\}$	
pg	$\{X, Y, P\}: \{P, PX\}$	The substitution of translation Y with antitranslation is forbidden.
	$\{P, Q\}: \{P, Q\}$	
$p4g$	$\{R_1, R_2, R_3, R_4, S\}: \{S\}\{R_1\}$	The simultaneous substitution of generators R_1, R_2, R_3, R_4 with antigenerators of the same kind of antisymmetry is obligatory.
	$\{R, S\}: \{R\}\{S\}$	
$p3$	$\{X, Y, Z, S_1\}$	The substitution of generators with antigenerators is forbidden.
	$\{S_1, S_2\}$	The substitution of generators with antigenerators is forbidden.
$p31m$	$\{S_1, S_2, R\}: \{R\}$	The substitution of generators S_1, S_2 with antigenerators is forbidden.
	$\{R, S\}: \{R\}$	The substitution of the generator S with antigenerators is forbidden.
$p3m$	$\{S_1, S_2, R\}: \{R\}$	The substitution of generators S_1, S_2 with antigenerators is forbidden.
	$\{R_1, R_2, R_3\}: \{R_1\}$	The simultaneous substitution of generators R_1, R_2, R_3 with antigenerators of the same kind of antisymmetry is obligatory.
$p6$	$\{S_1, S_2, T\}: \{T\}$	The subsitution of generators S_1, S_2 with antigenerators is forbidden.
	$\{S, T\}: \{T\}$	The substitution of the generator S with antigenerators is forbidden.
$p6m$	$\{R, R_1, R_2, R_3\}: \{R\}\{R_1\}$	The simultaneous substitution of generators R_1, R_2, R_3 with antigenerators of the same kind of antisymmetry is obligatory.
	$\{R, R_1, R_2\}: \{R\}\{R_1\}$	The simultaneous substitution of generators R_1, R_2 with antigenerators of the same kind of antisymmetry is obligatory.
cm	$\{P, Q, R\}: \{P\}\{R\}$	The simultaneous substitution of generators P, Q with antigenerators of the same kind of antisymmetry is obligatory.
	$\{P, R\}: \{P\}\{R\}$	
	$\{R, S\}: \{R\}\{S\}$	
pmm	$\{R, R', R_2, Y\}: \{\{R_2, R_2, Y\}, \{R, R'\}\}$	
	$\{R_1, R_2, R_3, R_4\}: \{\{R_1, R_3\}, \{R_2, R_4\}\}$	
pmg	$\{P, Q, R\}: \{R\}\{P, Q\}$	
	$\{T_1, T_2, R\}: \{R\}\{T_1, T_2\}$	
pgg	$\{P, Q, T\}: \{P, PT\}$	The simultaneous substitution of generators P, Q with antigenerators of the same kind of antisymmetry is obligatory.
	$\{P, O\}: \{P, O\}$	
cmm	$\{R_1, R_2, R_3, R_4, T\}: \{T\}\{R_1, R_2\}$	Generators R_1, R_3 and R_2, R_4 regarded in pairs demand a simultaneous substitution with antigenerators of the same kind of antisymmetry.
$p4$	$\{T_1, T_2, T_3, T_4, S\}: \{S, ST_1\}$	The simultaneous substitution of generators T_1, T_2, T_3, T_4 with antigenerators of the same kind of antisymmetry is obligatory.
	$\{S, T\}: \{S, ST\}$	
$p4m$	$\{R, R_1, R_2, R_3, R_4\}: \{R\}\{R_1, R_2\}$	Generators R_1, R_4 and R_2, R_3 regarded in pairs demand a simultaneous substitution with antigenerators of the same kind of antisymmetry.
	$\{R, R_1, R_2\}: \{R\}\{R_1, R_2\}$	

m fixed are generated within the same family from groups of the M^{m-1} type, $1 \leq m \leq l$.

Theorem 4: Groups of symmetry that possess isomorphic antisymmetric characteristics generate the same number of groups of M^m type for every fixed m, $1 \leq m \leq l$, which correspond to each other with regard to structure.

The presentations of the seventeen plane groups of symmetry, which are being used as generating groups, are given by Coxeter & Moser (1972).

In accordance with the definition above, the antisymmetric characteristics of the seventeen plane groups of symmetry have been defined and certain groups as well as their antisymmetric characteristics have been presented with two or several different presentations. The resulting antisymmetric characteristics are given on p. 210 and contain: the symbol of the symmetry group, the set of generators (Coxeter & Moser, 1972) and the reduced antisymmetric characteristic of the symmetry group as well as the conditions that result from the existential criterion - theorem 1.

The method of forming antisymmetric characteristics is illustrated with the example of the $p2$ group generated by translations X, Y and half-turn T. All products of generators formed in accordance with the definition can be divided into two classes of transformations equivalent with regard to symmetry (algebraic and geometric equivalent): translations X, Y, XY and half-turns T, TX, TY, TXY, so that the complete antisymmetric characteristic of this group is $\{X, Y, XY\}\{T, TX, TY, TXY\}$, the reduced form of which is $\{T, TX, TY, TXY\}$.

The catalogue of the plane groups of simple and multiple antisymmetry of the M^m type

For denoting the plane groups of simple and multiple antisymmetry of the M^m type, the 0-1 variant of the international symbols (Henry & Lonsdale, 1952) has been used in this study. The presence of the antiidentity of the ith kind ($1 \le i \le m$) within antigenerators has been marked with 1 on the ith position, from right to left. These 0-1 symbols correspond to the symbols used by Zamorzaev & Palistrant (1960) if the symbol _ is substituted by index 1, the symbol ′ by index 10, the symbol * by index 100, the symbol ^ by index 1000 (*e.g.* $*\hat{m}' = m_{1110}$, $\hat{\underline{m}} = m_{1001}$).

In accordance with theorem 4, the process of generating plane groups of simple and multiple antisymmetry of M^m type is enough to realize groups $p1$, $p2$, pm, pg, cm, pmm, $p31m$ with non-isomorphic antisymmetric characteristics. The method of generation is illustrated with the example of the group $p2\{X, Y, T\}$: $\{T, TX, TY, TXY\}$ which for $l=1$ generates groups of the M^1 type:

(1) $\{e_1X, Y, T\}((p_12)$, $\{X, e_1, Y, T\}(p_{0,1}2)$, $\{e_1X, e_1Y, T\}(p_{1,1}2)$, $\{e_1X, Y, e_1T\}(p_12_1)$, $\{X, e_1Y, e_1T\}(p_{0,1}2_1)$, $\{e_1X, e_1Y, e_1T\}(p_{1,1}2_1)$ with the antisymmetric characteristic $\{E, E, e_1, e_1\}$,†

(2) $\{X, Y, e_1T\}(p2_1)$ with antisymmetric characteristic $\{e_1, e_1, e_1, e_1\}$;

for $l=2$ generates groups of the M^2 type:

(1) $\{e_1X, e_2Y, T\}(p_{1,10}2)$, $\{e_1e_2X, e_2Y, T\}(p_{11,10}2)$, $\{e_1X, e_2Y, e_2T\}(p_{1,10}2_{10})$, $\{e_1e_2X, e_2Y, e_2T\}(p_{11,10}2_{10})$ with antisymmetric characteristic $\{E, e_1, e_2, e_1e_2\}$,

(2) $\{e_1X, Y, e_2T\}(p_12_{10})$ with antisymmetric characteristic $\{e_2, e_2, e_1e_2, e_1e_2\}$,

(3) $\{e_1e_2X, Y, e_2T\}(p_{11}2_{10})$ with antisymmetric characteristic $\{e_1, e_1, e_2, e_2\}$,

(4) $\{e_2X, Y, e_1T\}(p_{10}2_1)$, $\{X, e_2Y, e_1T\}(p_{0,10}2_1)$, $\{e_2X, e_2Y, e_1T\}(p_{10,10}2_1)$, $\{e_2X, Y, e_1e_2T\}(p_{10}2_{11})$, $\{X, e_2Y, e_1e_2T\}(p_{0,10}2_{11})$, $\{e_2X, e_2Y, e_1e_2T\}(p_{10,10}2_{11})$ with antisymmetric characteristic $\{e_1, e_1, e_1e_2, e_1e_2\}$;

for $l=3$ generates groups of the M^3 type:

(1) $\{e_1X, e_2Y, e_3T\}(p_{1,10}2_{100})$ with antisymmetric characteristic $\{e_3, e_1e_3, e_2e_3, e_1e_2e_3\}$,

(2) $\{e_1e_3X, e_2Y, e_3T\}(p_{101,10}2_{100})$ with antisymmetric characteristic $\{e_1, e_3, e_1e_2, e_2e_3\}$,

(3) $\{e_1X, e_2e_3Y, e_3T\}(p_{1,110}2_{100})$ with antisymmetric characteristic $\{e_2, e_3, e_1e_2, e_1e_3\}$,

(4) $\{e_1e_3X, e_2e_3Y, e_3T\}(p_{101,110}2_{100})$ with antisymmetric characteristic $\{e_1, e_2, e_3, e_1e_2e_3\}$,

(5) $\{e_1X, e_3Y, e_2T\}(p_{1,100}2_{10})$, $\{e_1e_3X, e_3Y, e_2T\}(p_{101,100}2_{10})$, $\{e_1X, e_3Y, e_2e_3T\}(p_{1,100}2_{110})$, $\{e_1e_3X, e_3Y, e_2e_3T\}(p_{101,100}2_{110})$ with antisymmetric characteristic $\{e_2, e_1e_2, e_2e_3, e_1e_2e_3\}$,

(6) $\{e_1e_2X, e_3Y, e_2T\}(p_{11,100}2_{10})$, $\{e_1e_2e_3X, e_3Y, e_2T\}(p_{111,100}2_{10})$, $\{e_1e_2X, e_3Y, e_2e_3T\}(p_{11,100}2_{110})$, $\{e_1e_2e_3X, e_3Y, e_2e_3T\}(p_{111,100}2_{110})$ with antisymmetric characteristic $\{e_1, e_2, e_1e_3, e_2e_3\}$,

(7) $\{e_2X, e_3Y, e_1T\}(p_{10,100}2_1)$, $\{e_2e_3X, e_3Y, e_1T\}(p_{110,100}2_1)$, $\{e_2X, e_3Y, e_1e_3T\}(p_{10,100}2_{101})$, $\{e_2e_3X, e_3Y, e_1e_3T\}(p_{110,100}2_{101})$ with antisymmetric characteristic $\{e_1, e_1e_2, e_1e_3, e_1e_2e_3\}$. For $l \ge 4$ the group $p2$, in accordance with theorem 1(b) does not generate groups of the M^m type, $m \ge 4$.

The final result of the generation is a complete catalogue of the plane groups of simple and multiple antisymmetry of M^m type, which consist of 46 groups of M^1 type, 167 groups of M^2 type, 700 groups of M^3 type and 2520 groups of M^4 type and which corresponds to the results given by Zamorzaev & Palistrant (1960).

† To shorten the marking with the antisymmetric characteristics we are giving only the antiidentities and their products that correspond to antigenerators.

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The Use of Non-Local Constraints in Maximum-Entropy Electron Density Reconstruction

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Abstract

Different expressions of the maximum-entropy estimates of the electron density function, corresponding to different prior information are obtained. They show that no general-purpose configurational entropy of density maps exists. Some universal properties of the modellings are discussed. In particular, the meaning of super-resolution is clarified. The information of lower and upper bounds of the electron density is not in general strong enough to produce atomic maps. Atomicity is then introduced as non-local constraints and applied to the problem of phase extension using experimental data and low-resolution model phases. In all cases, the knowledge of phases up to 3·5–3 Å and observed moduli up to 1·5–1 Å allows an estimate of the electron density of roughly the same quality as the 1 Å map obtained from a Fourier summation to be produced.

Introduction

The foundations of the theory here developed were given in a previous paper: the criterion of maximal entropy was used to obtain an estimate of the electron density function on the basis of partial information. First a maximum-entropy probability distribution of maps was obtained, its functional form being a strict consequence of the type of constraints used. Next the electron density function was estimated using this maximum-entropy probability distribution (Navaza, 1985).

For the particular type of constraint considered the formulation corresponds exactly to a maximum-entropy algorithm using new forms of the configurational entropy of maps and gives rise to a modelling of the maximum-entropy estimate of the sought map.

In this paper a slightly different presentation is offered aiming to show that no underlying probability distribution of maps is in fact needed in order to apply the recipes of information theory, even if we can always think in terms of frequencies in an idealized experimental situation. However, the probabilistic interpretation offers a conceptually simpler frame in which the problem of object reconstruction can be discussed.

Different developments of maximum entropy have been proposed and the references can be found in the previous paper. More recent developments are those of Bricogne (1984), Livesey & Skilling (1985) and Semenovskaya, Khachaturyan & Khachaturyan (1985). It is not the aim of this paper to discuss the different formulations.

Different modellings corresponding to different prior information are obtained and applied to experimental data. The results clearly showed that in the *ab initio* problem most maximum-entropy algorithms give uninterpretable maps. Moreover it was also found that the model phases (the 'true' phases) are not even placed in a concave region in the space of phases.

The problem of phase extension is also considered. Good results are obtained when information on atomicity is introduced in the form of non-local constraints. From the experimentally observed moduli corresponding to 1 Å resolution and the model phases up to 3·5–3 Å, all the atoms were recovered for structures with different numbers of atoms in the unit cell.

Finally, a critical discussion of super-resolution is presented. It is shown that, in general, little or no extra resolution of peaks is to be expected when most of the maximum-entropy algorithms are used.

Information and feasible maps

Crystallographers are faced with the problem of reconstructing a certain function ρ, taking values at

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