non-H independent protein atoms were determined, including 202 C, 55 N, 64 O and 6 S atoms. The globic scattering factors are used to calculate phases $\varphi_h(\text{glob})$ by means of (2). The phase error between the atomic and globic computed structure factors is

$$\Delta\varphi = \left(\sum_{\mathbf{h}} w_{\mathbf{h}}|\varphi_{\mathbf{h}}(\text{atom}) - \varphi_{\mathbf{h}}(\text{glob})|\right) \Big/ \left(\sum W_{\mathbf{h}}\right), \quad (5)$$

where $w_{\mathbf{h}} = |F_{\mathbf{h}0}|$ and $\varphi_{\mathbf{h}}(\text{atom})$ is the phase computed from the refined atomic coordinates. The average phase errors were calculated for resolution shells of 50 reflections, shown in Fig. 2. The error distribution clearly shows that the phase errors decrease rapidly when d's are longer than about 3.0 Å. A marked reduction of the globic phase error is achieved when the side-chain positions, in addition to the polypeptide backbone, have been modeled. Further reduction in phase error by modeling the ordered solvent structure is modest in comparison, *i.e.* less than 10°. Calculations performed for triclinic lysozyme, haemoglobin and erabutoxin reveal a similar pattern over the resolution range indicated in Fig. 2 (data not shown).

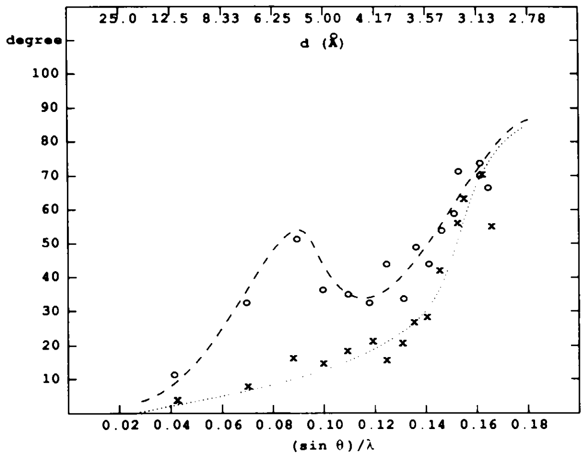

Fig. 2. Globic phase-error distribution of crambin. ····· Phasing by both main polypeptide-chain globs and side-chain globs. ----- Phasing by only polypeptide-chain globs. The peak in the latter curve at ~ 5.6 Å correlates well with the average closest separation distance between the side-chain globs of adjacent amino acid residues which were not included in the structure-factor calculation of the polypeptide-chain model.

In summary, globs may be advantageously used in low-resolution electron-density maps in which an atomic model cannot be confidently fitted.

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Non-magnetic twin laws.

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Abstract

Twin laws are groups that express the symmetry relationships between two simultaneously observed domain states (*domain pair*) and are used to determine physical properties that can distinguish between the observed domains. A tabulation is presented of all possible non-magnetic twin laws, that is, all possible *symmetry groups* and *twinning groups* of the domain pair. Additional information is provided related to determining twin laws. This includes the coset and double-coset decomposition of point groups, the indexing and point-group symmetry of domain states, permutations of domain states, and a classification of domain states.

1. Introduction

Crystalline domains can arise in phase transitions from a high-symmetry phase of symmetry **G** to a low-symmetry phase of symmetry **F**. The bulk structures of these domains in polydomain samples are referred to as *domain states*. Two domain states have the same crystal structure and differ only in their spatial orientation. Because of this difference in spatial orientation, when simultaneously observing two domain states, the two domain states can exhibit different physical properties (see *e.g.* Litvin & Litvin, 1990). In this paper, *domain states* will refer to *single-domain states* (Janovec, Richterova & Litvin, 1993), as we do not take into account any rotations of

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neighboring domains required for the neighboring domains to meet along a coherent domain wall. In the determination of the physical properties that can distinguish between simultaneously observed pairs of domain states (*domain pair*), the concept of *twin laws* has been introduced (Janovec, Richterova & Litvin, 1992). These laws are groups that express symmetry relationships from which one can determine the distinguishing physical properties of the domain pair, and depend on the symmetry of one domain state and the spatial relationship between the domain states. It has been shown that two types of twin law can be associated with a domain pair, the so-called *symmetry group* and the *twinning group* of the domain pair (Janovec & Fuksa, 1995; Janovec, Litvin & Fuksa, 1995). The symmetry group of a domain pair may allow one to express the order parameters and irreducible constituents of physical-property tensors in such a manner that their components in the two domains are either the same or differ only in sign. The twinning group determines which secondary order parameters are the same and which are different in the two domains of a domain pair. As only macroscopic physical properties are considered, the continuum description of the domain states is used and the analysis is based on point-group symmetry.

In this communication, we tabulate all possible non-magnetic twin laws. That is, for each point group $\mathbf{G}$ and each subgroup $\mathbf{F}$ of $\mathbf{G}$, we tabulate all possible domain-pair symmetry and twinning groups. In §2, we briefly review the concepts leading to and including twin laws. In §3, we detail the information contained in the tables of twin laws.

2. Twin laws

The number n of domain states that arise in a transition from a higher symmetry group $\mathbf{G}$ to a lower-symmetry group $\mathbf{F}$ is $n = |\mathbf{G}|/|\mathbf{F}|$, where $|\mathbf{A}|$ denotes the order of group $\mathbf{A}$. There is a one-to-one correspondence between the n domain states $S(i)$, $i = 1, 2, ..., n$ and the cosets $g_i\mathbf{F}$, $i = 1, 2, ..., n$, of the coset decomposition of $\mathbf{G}$ with respect to $\mathbf{F}$:

$$\mathbf{G} = g_1\mathbf{F} + g_2\mathbf{F} + g_3\mathbf{F} + \ldots + g_n\mathbf{F}. \quad (1)$$

$S(i) = g_iS(1)$, where g_i is the ith coset representative of the coset decomposition. The domain state $S(1)$ is invariant under $\mathbf{F}_1 \equiv \mathbf{F}$ and $S(i)$ under $\mathbf{F}_i = g_i\mathbf{F}g_i^{-1}$.

A domain pair is denoted by $\{S(i), S(j)\}$. The n^2 domain pair can be partitioned into classes: two domain pairs $\{S(i), S(j)\}$ and $\{S(i'), S(j')\}$ are defined to be in the same class of domain pairs if there exists an element g of $\mathbf{G}$ such that $\{S(i'), S(j')\} = \{gS(i'), gS(j')\}$. The number m of classes of domain pairs is equal to the number of double cosets in the double-coset decomposition of $\mathbf{G}$ with respect to $\mathbf{F}$ (Janovec, 1972):

$$\mathbf{G} = \mathbf{F}g_1^{dc}\mathbf{F} + \mathbf{F}g_2^{dc}\mathbf{F} + \ldots + \mathbf{F}g_m^{dc}\mathbf{F}. \quad (2)$$

A single representative domain pair from each class of domain pairs can be chosen as $\{S(1), g_i^{dc}S(1)\}$, $i = 1, 2, \ldots, m$, where g_i^{dc} is the ith double-coset representative of the double-coset decomposition.

The symmetry group $\mathbf{J}_{ij}$ of the domain pair $\{S(i), S(j)\}$ is defined by

$$\mathbf{J}_{ij} = \mathbf{F}_{ij} + g_{ij}^{*}\mathbf{F}_{ij}, \quad (3)$$

where $\mathbf{F}_{ij} = \mathbf{F}_i \cap \mathbf{F}_j$ consists of all elements of $\mathbf{G}$ that simultaneously leave domain states $S(i)$ and $S(j)$ invariant and $g_{ij}^{*}S(i) = S(j)$ and $g_{ij}^{*}S(j) = S(i)$. g_{ij}^{*} interexchanges the two domain states $S(i)$ and $S(j)$. If no such element g_{ij}^{*} exists, then $\mathbf{J}_{ij} = \mathbf{F}_{ij}$. Only in the former case, where the domain pair is referred to as transposable, can this group be used to express the irreducible constituents of physical-property tensors in such a manner that their components in the two domains are either the same or differ only in sign (Janovec, Richterova & Litvin, 1992, 1993; Janovec, Litvin & Richterova, 1994).

The twinning group $\mathbf{K}_{ij}$ of a domain pair $\{S(i), S(j)\}$ is defined by

$$\mathbf{K}_{ij} = \langle \mathbf{F}_i, g_{ij} \rangle, \quad (4)$$

where $\mathbf{F}_i$ is the point group of $S(i)$ and $g_{ij}S(i) = S(j)$. g_{ij} transforms the domain state $S(i)$ into the domain state $S(j)$. The twinning group $\mathbf{K}_{ij}$ is the group generated by the elements

Table 1. *Coset and double-coset decomposition of* $\mathbf{G} = \mathbf{6mm}$ *with respect to* $\mathbf{F} = \mathbf{m}_x$*: each row contains the elements of a single coset, sets of cosets constituting a single double coset are separated by a rule*

1	m_x
6_z	m_1
m_3	6_z^5
3_z	m_{xy}
m_y	3_z^2
2_z	m_2

Table 2. *Index i and point-group symmetry* $\mathbf{F}_i$ *of the domain states* $S(i)$ *in the caseof* $\mathbf{G} = \mathbf{6mm}$ *and* $\mathbf{F} = \mathbf{m}_x$

Index	$S_i = g_iS_1$	$\mathbf{F}_i = g_i\mathbf{F}_1g_i^{-1}$
1	$S_1 = 1S_1$	$\mathbf{F}_1 = \mathbf{m}_x$
2	$S_2 = 6_zS_1$	$\mathbf{F}_2 = \mathbf{m}_{xy}$
3	$S_3 = m_3S_1$	$\mathbf{F}_3 = \mathbf{m}_y$
4	$S_4 = 3_zS_1$	$\mathbf{F}_4 = \mathbf{m}_y$
5	$S_5 = m_yS_1$	$\mathbf{F}_5 = \mathbf{m}_{xy}$
6	$S_6 = 2_zS_1$	$\mathbf{F}_6 = \mathbf{m}_x$

Table 3. *Permutations of the domain states* $S(i)$ *under the action of elements* g *of* $\mathbf{G}$ *in the case of* $\mathbf{G} = \mathbf{6mm}$ *and* $\mathbf{F} = \mathbf{m}_x$

Element of G	Permutation	Element of G	Permutation
1	123456 123456	m_x	123456 132546
6_z	123456 241635	m_1	123456 214365
3_z	123456 462513	m_{xy}	123456 426153
2_z	123456 654321	m_2	123456 645231
3_z^2	123456 536142	m_y	123456 563412
6_z^5	123456 315264	m_3	123456 351624

Table 4. *Classes of domain pair in the case of* $\mathbf{G} = \mathbf{6mm}$ *and* $\mathbf{F} = \mathbf{m}_x$

1	$\{S(1), S(1)\}$	$\{S(2), S(2)\}$	$\{S(3), S(3)\}$	$\{S(4), S(4)\}$	$\{S(5), S(5)\}$	$\{S(6), S(6)\}$
2	$\{S(1), S(2)\}$	$\{S(2), S(4)\}$ $\{S(1), S(3)\}$ $\{S(3), S(5)\}$	$\{S(4), S(6)\}$ $\{S(2), S(1)\}$	$\{S(6), S(5)\}$ $\{S(4), S(2)\}$	$\{S(5), S(3)\}$ $\{S(6), S(4)\}$	$\{S(3), S(1)\}$ $\{S(5), S(6)\}$
3	$\{S(1), S(4)\}$	$\{S(2), S(6)\}$ $\{S(1), S(5)\}$ $\{S(3), S(6)\}$	$\{S(4), S(5)\}$ $\{S(2), S(3)\}$	$\{S(6), S(3)\}$ $\{S(4), S(1)\}$	$\{S(5), S(1)\}$ $\{S(6), S(2)\}$	$\{S(3), S(2)\}$ $\{S(5), S(4)\}$
4	$\{S(1), S(6)\}$	$\{S(2), S(5)\}$	$\{S(4), S(3)\}$	$\{S(6), S(1)\}$	$\{S(5), S(2)\}$	$\{S(3), S(4)\}$

of $\mathbf{F}_i$ and the element g_{ij}, *i.e.* the smallest subgroup of $\mathbf{G}$ which contains both $\mathbf{F}_i$ and the element g_{ij}.

3. Twin law tabulations

The computer-generated information available in the twin law tabulations consists of the following:*

(1) Coset and double-coset decomposition of the point group $\mathbf{G}$ with respect to a subgroup $\mathbf{F}$ of $\mathbf{G}$ (Janovec, Dvorakova, Wike & Litvin, 1989). For example, in Table 1 we list the coset and double-coset decomposition of $\mathbf{G} = \mathbf{6mm}$ with respect to the subgroup $\mathbf{F} = \mathbf{m}_x$. Each row in the table lists the elements of each of the $|\mathbf{G}|/|\mathbf{F}| = 12/2 = 6$ cosets. The coset representatives g_i, $i = 1, 2, \ldots, 6$, see (1), can be taken as the first element in each row. Sets of cosets separated by rules constitute the double cosets of the double-coset decomposition of $\mathbf{G}$ with respect to $\mathbf{F}$. In Table 1, we have four double cosets and the double-coset representatives g_i^{dc}, $i = 1, 2, 3, 4$, can be taken as the first element of the first coset in each of the double cosets.

(2) Indexing and point-group symmetry of the domain states. The domain state $S(i)$ is defined by $S(i) = g_iS(1)$, where g_i is the ith coset representative and $S(1)$ is the domain-state invariant under $\mathbf{F}$. The point group $\mathbf{F}_i$ of the domain $S(i)$ is defined by $\mathbf{F}_i = g_i\mathbf{F}g_i^{-1}$. For $\mathbf{G} = \mathbf{6mm}$ and $\mathbf{F} = \mathbf{m}_x$, the indexing and point-group symmetry of the domain states are given in Table 2.

(3) Permutations of the domain states. We determine the permutations of the domain states under the action of each element g of the group $\mathbf{G}$, *i.e.* for each element g of $\mathbf{G}$ and each domain $S(i)$, we tabulate $S(j) = gS(i)$. For $\mathbf{G} = \mathbf{6mm}$ and $\mathbf{F} = \mathbf{m}_x$, we give these permutations in Table 3. Next to each element g of $\mathbf{G}$ we give the permutation

$$\begin{array}{c} S(1)\; S(2)\; \ldots\; S(n) \\ gS(1)\; gS(2)\; \ldots\; gS(n), \end{array}$$

where, for typographical simplicity, only the indices of the domain states $S(i)$ and $S(j) = gS(i)$ are explicitly listed.

(4) Classes of domain pairs. The number of classes of domain pairs is equal to the number of double cosets in the double-coset decomposition of $\mathbf{G}$ with respect to $\mathbf{F}$. A representative domain pair from each class can be chosen as the domain pair $\{S(1), g_i^{dc}S(1)\}$. For $\mathbf{G} = \mathbf{6mm}$ and $\mathbf{F} = \mathbf{m}_x$, the four classes of domain pairs are listed in Table 4. The first domain pair of each class is the representative domain pair $\{S(1), g_i^{dc}S(1)\}$.

(5) Twin laws. For every point group $\mathbf{G}$, subgroup $\mathbf{F}$ and representative domain pair $\{S(1), g_i^{dc}S(1)\}$, except for $i = 1$, we tabulate the domain pair's symmetry group, (3), and twinning group, (4). The case $i = 1$ is not considered as the corresponding domain pair $\{S(1), S(1)\}$ consists of identical domain states. We consider only one domain pair from each class because the relative spatial orientation is the same for the two domain states in each domain pair of a single class (Litvin & Wike, 1989). For $\mathbf{G} = \mathbf{6mm}$ and $\mathbf{F} = \mathbf{m}_x$, the twin laws are given in Table 5.

Table 5. *The symmetry group* $\mathbf{J}_{1j}$ *and twinning group* $\mathbf{K}_{1j}$ *of the representative domain pair* $\{S(1), S(j)\}$ *in the case* $\mathbf{G} = \mathbf{6mm}$ *and* $\mathbf{F} = \mathbf{m}_x$

Representative domain pair $\{S(1), S(j)\}$	$\mathbf{J}_{1j}$ $\mathbf{K}_{1j}$	$\mathbf{F}_{1j}$ $\mathbf{F}_1$	g_{1j}^* g_{1j}
$\{S(1), S(2)\}$	$\mathbf{m}_1$ $\mathbf{6mm}$	$\mathbf{1}$ $\mathbf{m}_x$	m_1 6_z
$\{S(1), S(4)\}$	$\mathbf{m}_{xy}$ $\mathbf{3}_z\mathbf{m}_x$	$\mathbf{1}$ $\mathbf{m}_x$	m_{xy} 3_z
$\{S(1), S(6)\}$	$\mathbf{m}_x\mathbf{m}_2\mathbf{2}_z$ $\mathbf{m}_x\mathbf{m}_2\mathbf{2}_z$	$\mathbf{m}_x$ $\mathbf{m}_x$	2_z 2_z

(6) Additional options provide the user with complete flexibility in choosing which domain pair to consider in determining domain-pair twin laws. The symmetry group and twinning group of domain pair $\{S(1), gS(1)\}$, where g is an arbitrary element of $\mathbf{G}$, and of domain pair $\{S(i), S(j)\}$, for arbitrary domain states $S(i)$ and $S(j)$, can also be calculated.

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* A computer program for IBM-compatible computers entitled *Non-Magnetic Twin Laws* has been deposited with the IUCr [Reference: CR0499 (1 disk)]. Copies are available through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. For a given point group $\mathbf{G}$ and subgroup $\mathbf{F}$, this program calculates the coset decomposition of $\mathbf{G}$ with respect to $\mathbf{F}$, the indices and point group of the domain states, the permutations of the domains, classes of domain pairs, and the symmetry and twinning groups of representative domain pair, domain pair $\{S(1), gS(1)\}$ and arbitrary domain pair $\{S(i), S(j)\}$.

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