Table 3. *Examples of equivalent superspace groups*

The first column indicates some space groups as they are listed in Table 2 of I. The remaining columns are the equivalent groups obtained from those in the first column by employing the wave vector shown in the heading.

$\mathbf{q}=\gamma\mathbf{c}^*$	$\mathbf{q}=(\gamma-1)\mathbf{c}^*$	$\mathbf{q}=(\gamma-2)\mathbf{c}^*$	$\mathbf{q}=(\gamma-3)\mathbf{c}^*$
$P^{P\,m\,c\,n}_{\;\;s\,1\,\bar{1}}$	$P^{P\,m\,c\,n}_{\;\;s\,s\,\bar{1}}$		
$P^{P4_1 2 2}_{\;\;1\,\bar{1}\,\bar{1}}$	$P^{P4_1 2 2}_{\;\;q\,\bar{1}\,\bar{1}}$	$P^{P4_1 2 2}_{\;\;s\,\bar{1}\,\bar{1}}$	
$P^{P6_1}_{\;\;1}$	$P^{P6_1}_{\;\;h}$	$P^{P6_1}_{\;\;t}$	$P^{P6_1}_{\;\;s}$
$P^{F\,d\,d\,2}_{\;\;1\,1\,1}$	$P^{F\,d\,d\,2}_{\;\;q\,q\,1}$	$P^{F\,d\,d\,2}_{\;\;s\,s\,1}$	
$P^{I4_1/a}_{\;\;1\;\;\bar{1}}$	$P^{I4_1/a}_{\;\;q\;\;\bar{1}}$	$P^{I4_1/a}_{\;\;s\;\;\bar{1}}$	

1, s, t, q or h is written in the bottom line. For superspace groups with non-zero $\mathbf{q}_r$, which are denoted by A, B, C, L, M, N, U, V, W and R in the prefix of the symbol, several values of τ are possible. For example, we consider $A^{P\,m\,m\,m}_{\;\;1\,1\,\bar{1}}$, which has $\mathbf{q}_r=\mathbf{a}^*/2$. By the convention in I, the first $\binom{m}{1}$ represents a (hyper-) mirror plane perpendicular to the a axis with $\tau=0$. On the other hand, the same group also has a mirror plane parallel to this but a distance $a/2$ apart because of the lattice translation $\mathbf{a}$. The value of τ corresponding to the latter is then $\frac{1}{2}$. Hence the symbol for this plane is $\binom{m}{s}$. Thus $A^{P\,m\,m\,m}_{\;\;s\,1\,\bar{1}}$ represents the same group as $A^{P\,m\,m\,m}_{\;\;1\,1\,\bar{1}}$. This is analogous to the situation in three dimensions, where, for example, *Ammm* could also be written as *Ancb*. However, conventions such as those that give preference to *Ammm* have not yet been formulated for superspace groups. Notice that, just as in the three-dimensional case, the non-uniqueness of the symbol does not play a role in the reflection conditions and is of no practical consequence.

4. Equivalent superspace groups

The $\mathbf{q}$ dependence of the superspace group symbol is related to the equivalence of superspace groups. For example, consider $P^{P\,m\,c\,n}_{\;\;s\,s\,\bar{1}}$ with $\mathbf{q}=\gamma\mathbf{c}^*$, which is the superspace group appearing in the incommensurate phase of K_2SeO_4 (Janner & Janssen, 1980). For the choice $\mathbf{q}=(\gamma-1)\mathbf{c}^*$, the superspace group becomes $P^{P\,m\,c\,n}_{\;\;s\,1\,\bar{1}}$ because δ is invariant and $\mathbf{q}_r$ is $-\mathbf{c}^*$ in this case. Thus a different choice of $\mathbf{q}$ may lead to a different superspace group. This is however always equivalent to the original one (Janner & Janssen, 1979). For the sake of the practical problem encountered in the determination of the superspace group, several examples of equivalent superspace groups are shown in Table 3.

In addition, there are many equivalent superspace groups that are related to the choice of the basic vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$. Consider again $P^{P\,m\,c\,n}_{\;\;s\,s\,\bar{1}}$. This is equivalent to $P^{P\,n\,a\,m}_{\;\;\bar{1}\,s\,s}$: the latter is obtained from the former by exchanging the a and c axes. Such a kind of equivalence relation is similar to that in the usual space groups.

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Space Groups of Coincidence-Site Lattice Dichromatic Patterns in the Cubic System

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Abstract

The determination of the full space symmetry of two interpenetrating lattices in a coincidence-site lattice orientation is discussed. The considered coincidence-site lattices are formed by two primitive cubic, face-centred cubic or body-centred cubic lattices. The two interpenetrating lattices form a dichromatic pattern and its symmetry is investigated by combining the three-dimensional periodicity of the coincidence-site lattice with the point-symmetry operations of the motif characterizing the particular dichromatic pattern. This provides a very concise formulation for treating this subject, especially if antisymmetry (two-coloured symmetry) is used. The translational symmetry of coincidence-site lattices with $\Sigma<50$ is specified by determining the finest common sublattice of the two interpenetrating lattices. The point symmetry is determined by using the principle of the symmetry of composites and it is shown that the

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permissible point groups of dichromatic patterns in the cubic system are $4/mm'm'$, $6'/m'mm'$, $\bar{3}m'$, $mm'm'$, $2'/m'$, $\bar{1}$.

1. Introduction

The coincidence-site lattice is the most commonly used model for describing the geometry of grain boundaries. Working with this model we consider two interpenetrating lattices so that they have at least one point in common, which is called a coincidence site, and choose that point as origin. Depending on the metric properties of the lattices and on their relative orientation, more coincidence sites may exist and these extra sites may exhibit one-, two- or three-dimensional periodicity. In the last case we speak of a coincidence-site lattice (CS lattice or CSL).

In recent papers (Pond & Bollmann, 1979; Pond & Vlachavas, 1983) the symmetry of CS lattices has been discussed by introducing the concept of the dichromatic pattern. This is the pattern created by two interpenetrating lattices forming the CSL; one of the lattices is regarded as white and the other as black. The symmetry of the dichromatic pattern is then described in terms of two-coloured symmetry (or antisymmetry) elements (Shubnikov & Koptsik, 1977). In this respect, the black and white lattices are invariant with respect to ordinary symmetry operations, but they are mutually transformed (*i.e.* black to white and *vice versa*) by the colour-reversing symmetry operations.

The dichromatic pattern describes the spatial distribution of the points of the black and white lattices as well as the geometrical interrelations existing between these points. Thus, it exhibits two distinct features: the recurring motif, which indicates some grouping of white and black lattice points, and the way this motif is repeated throughout the space (Pond & Vlachavas, 1983). The spatial repetition of the motif is conveniently specified by means of the CS lattice, which is, by definition, the finest common sublattice of the black and white lattices. The CS lattice is a mathematical construction, which is introduced and studied quite independently of the motif structure of a dichromatic pattern. Accordingly, the determination of the space symmetry of a dichromatic pattern can be accomplished in stages by (a) finding the translation group of the CS lattice, (b) establishing the point symmetry consistent with the motif that characterizes the particular dichromatic pattern, and (c) combining the translational and point symmetries.

This paper will specifically be devoted to the determination of the symmetry groups of three-dimensional periodic dichromatic patterns (CSL dichromatic patterns) formed by two metrically identical cubic lattices. For this, the relative orientation (misorientation) of the two lattices is restricted to those values only that correspond to a CSL orientation. The misorientation is described by a rotation angle θ along an axis $[uvw]$, where $[uvw]$ is expressed in the coordinate system of the white lattice, which is kept fixed in space. This coordinate system is orthogonal right-handed having its origin on a coincidence site, its axes parallel to the edges of a standard cubic unit cell of the white lattice and we choose the length of an edge as the length unit.

2. Coincidence-site lattice misorientations

Axis/angle pairs, $[uvw]/\theta$, describing rotations that bring the white and the black lattices in partial coincidence (CSL misorientations) have been reported in many papers (Ranganathan, 1966; Warrington & Bufalini, 1971; Bruggeman, Bishop & Hartt, 1972; Fortes, 1972; Grimmer, 1973; Grimmer, Bollmann & Warrington, 1974; Bleris, Antonopoulos, Karakostas & Delavignette, 1981). Any CSL misorientation is characterized, except for the parameters $[uvw]$ and θ, by an integral number, Σ, which is the ratio of volumes of the primitive unit cells of the CSL and the white (or black) lattice and is unique for each CS lattice. Grimmer (1974) has shown that a CS lattice corresponding to a given value of Σ can be, in general, expressed by more than one symmetry-equivalent orientation relationship.

In the case of cubic lattices there are 24 equivalent descriptions of a CSL misorientation and one of them is chosen as representative of the particular CS lattice. However, this selection is not completely arbitrary. Usually, we use as standard description that one corresponding to the smallest positive value of the rotation angle consistent with the considered CSL (smallest-angle description). Alternatively, as pointed out by Fortes (1972), most of the CSL misorientations can be expressed in terms of a 180° rotation (180° angle description). In some instances, however, it is important to know whether or not a given CSL misorientation can be described in terms of a rotation about a symmetry axis of the white lattice. For this purpose, we use in the present work a third description of the CSL misorientations. It is completely equivalent to the previous descriptions and is introduced only for those CSL misorientations for which the smallest-angle description does not correspond to a rotation about the [100], [110] and [111] directions of the white lattice. The new description specifies a CSL misorientation by the axis/angle pair corresponding to the minimum value $u^2+v^2+w^2$ of the rotation axes $[uvw]$ consistent with the particular CSL (low-index description). If more than one axis/angle pair fulfils the above criterion then the axis/angle pair with the smaller rotation angle is taken as the low-index description. The smallest-angle descriptions of CSL rotations about [100], [110] or [111] and their corresponding low-index descriptions are taken to be identical.

Table 1 lists the three alternative descriptions of CSL misorientations in the cubic system with $\Sigma < 50$. The tabulated rotation axes lie within the standard stereographic triangle [100]-[110]-[111]. The different Σ corresponding to the same multiplicity (same Σ value) are classified alphabetically starting with the description having the smallest rotation angle. As can be seen, only the $\Sigma = 39b$ CSL misorientation cannot be reduced to a 180° rotation relationship (Fortes, 1972).

3. Symmetry operations of CSL dichromatic patterns

The purpose of this section is to analyse the principles for the determination of the three-dimensional periodicity of a CS lattice and the point symmetry consistent with the motif of the corresponding dichromatic pattern. We designate the antisymmetry space group of the CSL dichromatic pattern by $\boldsymbol{\Psi}(p)$; it can be expressed in matrix operator terms as (Pond & Vlachavas, 1983)

$$\boldsymbol{\Psi}(p) = \{[\mathsf{D}(o)_i|\boldsymbol{\tau}_i] \cup [\mathsf{D}(c)_i|\boldsymbol{\tau}_i]\}$$
$$\leftrightarrow \{\mathbf{T}(p)([\mathsf{D}(o)_i|\mathbf{0}] \cup [\mathsf{D}(c)_i|\mathbf{0}])\},$$

where $\mathbf{T}(p) = \{[\mathsf{E}|\boldsymbol{\tau}_i]\}$ and E is the matrix representing the (ordinary) identity symmetry operation. $\mathbf{T}(p)$ is the group of (ordinary) translation vectors of the CS lattice. $\mathsf{D}(o)_i$ and $\mathsf{D}(c)_i$ are the matrix representations of the ordinary and colour-reversing point-symmetry operations, respectively.

This expression indicates that the antisymmetry space group of a CSL dichromatic pattern is always symmorphic and, consequently, $\boldsymbol{\Psi}(p)$ is determined by combining directly the translations in the group $\mathbf{T}(p)$ with all point-symmetry operations of the types $\mathsf{D}(o)_i$ and $\mathsf{D}(c)_i$.

The three-dimensional translational symmetry of a CS lattice is investigated by considering the geometrical relationship between the black and the white lattices. Denoting by $\mathbf{T}(\mu) = \{[\mathsf{E}|\boldsymbol{\tau}(\mu)_i]\}$ and $\mathbf{T}(\lambda) = \{[\mathsf{E}|\boldsymbol{\tau}(\lambda)_i]\}$ the translation groups of the black and white lattices, respectively, we have that the group $\mathbf{T}(p)$ is given by the intersection $\mathbf{T}(p) = \mathbf{T}(\lambda) \cap \mathbf{T}(\mu)$. Consequently, the group $\mathbf{T}(p)$ is equivalent to the set of white lattice vectors that satisfy the relation (Pond & Vlachavas, 1983)

$$\boldsymbol{\tau}(\lambda)_j = \mathsf{R}\boldsymbol{\tau}(\lambda)_i, \qquad (1)$$

where R is the coordinate transformation describing the rotation of the black lattice relative to the white (Warrington & Bufalini, 1971).

The determination of the point group of a dichromatic pattern is based on the principle of composite symmetry and, accordingly, the point-symmetry operations can be directly found by superposing the black and white point groups so that they have common origin (Vlachavas, 1984).

Table 1. *The CSL misorientations in the cubic system with $\Sigma < 50$ are expressed by their smallest-angle,* 180° *angle and low-index descriptions*

The rotation axes $[uvw]$ are taken in the standard stereographic triangle ($u \geq v \geq w \geq 0$). For the sake of simplicity, the square brackets in the symbols of rotation axes have been omitted.

Σ	Smallest-angle description	180° angle description		Low-index description
3	111/60°	111	211	
5	100/36·87°	210	310	
7	111/38·21°		321	
9	110/38·94°	221	411	
11	110/50·48°	311	332	
13*a*	100/22·62°	320	510	
13*b*	111/27·80°		431	
15	210/48·19°		521	
17*a*	100/28·07°	410	530	
17*b*	221/61·93°	322	433	110/86·63°
19*a*	110/26·53°	331	611	
19*b*	111/46·83°		532	
21*a*	111/21·79°		541	
21*b*	211/44·42°	421		210/58·41°
23	311/40·46°		631	210/163·04°
25*a*	100/16.26°	430	710	
25*b*	331/51·68°		543	211/156·93°
27*a*	110/31·59°	511	552	
27*b*	210/35·43°		721	
29*a*	100/43·60°	520	730	
29*b*	221/46·40°	432		210/112·29°
31*a*	111/17·90°		651	
31*b*	211/52·20°		732	
33*a*	110/20·05°	441	811	
33*b*	311/33·56°		741	211/117·04°
33*c*	110/58·99°	522	554	
35*a*	211/34·05°	531		
35*b*	331/43·23°		653	210/106·60°
37*a*	100/18·92°	610	750	
37*b*	310/43·14°		831	221/161·08°
37*c*	111/50·57°		743	
39*a*	111/32·20°		752	
39*b*	321/50·13°			
41*a*	100/12·65°	540	910	
41*b*	210/40·88°	621		
41*c*	110/55·88°	443	833	
43*a*	111/15·18°		761	
43*b*	210/27·91°		921	
43*c*	332/60·77°	533	655	110/80·63°
45*a*	311/28·62°		851	221/126·87°
45*b*	221/36·87°	542		210/83·62°
45*c*	221/53·13°		754	
47*a*	331/37·07°		763	210/87·56°
47*b*	320/43·66°		932	310/156·19°
49*a*	111/43·57°		853	
49*b*	511/43·57°		941	211/88·83°
49*c*	322/49·23°	632		210/146·80°

4. Point groups for CSL rotations in the cubic lattices

In the case of CSL dichromatic patterns the rotation matrix R corresponds to known misorientation relationships (Table 1) and, consequently, the determination of the point-symmetry operations can be formulated in a concise algorithm (Vlachavas, 1984). We denote by $\mathbf{D}_\lambda$ and $\mathbf{D}_\mu$ the point groups of the white and black lattices, respectively, and by $\mathsf{D}(\lambda)_i$, $i = 1, 2, \ldots, r_\lambda$, the operations of $\mathbf{D}_\lambda$, where r_λ is the order of $\mathbf{D}_\lambda$. For the dichromatic patterns considered in the present work we have $\mathbf{D}_\lambda \equiv \mathbf{D}_\mu = m3m$. The set

$\mathbf{D}_o$ of the ordinary operations $\mathsf{D}(o)_i$ of the dichromatic pattern is obtained by forming the products* $\mathsf{R}^{-1}\mathsf{D}(\lambda)_i\mathsf{R}$, $i=1,2,\ldots,r_\lambda$, and taking only those symmetry operations of the white point group for which $\mathsf{R}^{-1}\mathsf{D}(\lambda)_i\mathsf{R}\in\mathbf{D}_\lambda$; thus, $\mathbf{D}_o$ is an order r subgroup of $\mathbf{D}_\lambda$. Next, we examine the form of the rotation R. If $\mathsf{R}^2\in\mathbf{D}_o$, the point group of the CSL dichromatic pattern is given by $\mathbf{D}=\mathbf{D}_o+\mathbf{D}_o\mathsf{R}$. Otherwise, we take all the factor 2 supergroups of $\mathbf{D}_o$ that are subgroups of $\mathbf{D}_\lambda$ and we denote them by $\mathbf{D}_{2,i}=\{\mathsf{D}(o)_1, \mathsf{D}(o)_2,\ldots,\mathsf{D}(o)_r, \mathsf{D}'(\lambda)_1, \mathsf{D}'(\lambda)_2,\ldots,\mathsf{D}'(\lambda)_r\}$. For each $\mathbf{D}_{2,i}$ we form the products $\mathsf{D}'(\lambda)_i\mathsf{R}\mathsf{D}'(\lambda)_i\mathsf{R}$, $i=1,2,\ldots,r$. If $\mathsf{D}'(\lambda)_i\mathsf{R}\mathsf{D}'(\lambda)_i\mathsf{R}\in\mathbf{D}_o$, then the dichromatic point group is $\mathbf{D}=\mathbf{D}_o+\{\mathsf{D}'(\lambda)_1\mathsf{R}, \mathsf{D}'(\lambda)_2\mathsf{R},\ldots,\mathsf{D}'(\lambda)_r\mathsf{R}\}$, whereas if $\mathsf{D}'(\lambda)_i\mathsf{R}\mathsf{D}'(\lambda)_i\mathsf{R}\notin\mathbf{D}_o$ for all $\mathsf{D}'(\lambda)_i\in\{\mathbf{D}_{2,i}-\mathbf{D}_o\}$ and all subgroups $\mathbf{D}_{2,i}$, the dichromatic point group is $\mathbf{D}_o$.

Before applying this algorithm, it is of interest to notice that the rotation matrix R, expressed in the coordinate system of the white lattice, represents an orthogonal transformation and, hence, $\mathsf{R}^{-1}\mathsf{E}\mathsf{R}=\mathsf{E}$ and $\mathsf{R}^{-1}\mathsf{i}\mathsf{R}-\mathsf{i}$, where i is the matrix representing the inversion symmetry operation. An immediate consequence is that $\mathbf{D}_o$ corresponds always to a centrosymmetric point group and, therefore, $\mathbf{D}_o$ can only be one of the following subgroups of $\mathbf{D}_\lambda=m3m$: $\bar{1}$, $2/m$, mmm, $4/m$, $4/mmm$, $\bar{3}$, $\bar{3}m$, $m3$, $m3m$.

Also, we note that the algorithm simplifies considerably when the transformation R^2 is equivalent to a symmetry operation of the white point group. For the CSL rotations in Table 1, with the exception of $\Sigma=39b$, the point group of the associated dichromatic pattern is expressed as $\mathbf{D}=\mathbf{D}_o+\mathbf{D}_o2^{1'}$, where $2^{1'}$ is the twofold colour-reversing operation equivalent to the 180° description of the CSL rotation. For determining the point group $\mathbf{D}$ we consider four distinct categories of 180° CSL rotations.

The first category contains the 180° rotations along $[uv0]$. The symmetry elements of the white point group that are invariant with respect to these rotations form the point group $\mathbf{D}_o=4/m$. This can be easily seen by noting that relation $\mathsf{D}(\lambda)_i=\mathsf{R}^{-1}\mathsf{D}(\lambda)_j\mathsf{R}$ only holds for those symmetry elements that are either parallel or perpendicular to the rotation axis.† Thus, the point groups of the dichromatic patterns for the $[uv0]/180°$ rotations are isomorphic to $\mathbf{D}=\mathbf{D}_o+\mathbf{D}_o2^{1'}_{uv0}=\{4/m\}+\{4/m\}2^{1'}_{uv0}=4/mm'm'$ [for the notation of symmetry operations see Vlachavas (1984)].

The second category comprises the 180° rotations along a direction of the general form $[v+w, v, w]$; they are alternatively described as $[111]/\theta$ (Table 1). All these misorientations, except the $\Sigma=3$ $[111]/60°\equiv[111]/180°\equiv[211]/180°$ (see below), lead to CSL dichromatic patterns in which the ordinary symmetry operations form the $\mathbf{D}_o=\bar{3}$ group. Consequently, these patterns possess point symmetry expressed by $\mathbf{D}=\{\bar{3}\}+\{\bar{3}\}2^{1'}_{v+w,v,w}=\bar{3}m'$ with $v>w>0$.

In the third category we have rotations of 180° along a direction of the general form $[uuw]$ or $[uvv]$. For these we have $\mathbf{D}=\{2/m\}+\{2/m\}2^{1'}_{uuw}=\{2/m\}+\{2/m\}2^{1'}_{uvv}=mm'm'$. The remaining 180° rotations belong in the fourth category and they yield dichromatic patterns with $\mathbf{D}_o=\bar{1}$ and, thus, the point group $\mathbf{D}$ is expressed by $\mathbf{D}=\{\bar{1}\}+\{\bar{1}\}2^{1'}_{uvw}=2'/m'$.

The $\Sigma=3$ misorientation represents a special case as far as the symmetry of the dichromatic pattern is concerned. In fact, it is the only CSL rotation in the cubic system giving dichromatic patterns with point symmetry non-isomorphic to a subgroup of the group $\mathbf{D}_\lambda\equiv\mathbf{D}_\mu=m3m$. The lowest-angle description of the $\Sigma=3$ rotation is $[111]/60°$ and it corresponds to the symmetry operation $6^{1'}_{111}$. The combination of $6^{1'}_{111}$ with the threefold ordinary symmetry axis parallel to [111] yields a sixfold colour-reversing axis (Vlachavas, 1984). In group-theoretical terms, we note that for the $[111]/60°$ rotation the group of the ordinary operations is $\mathbf{D}_o=\bar{3}m$, with $\bar{3}$ parallel to [111] and, accordingly, $\mathbf{D}$ is obtained by the extension $\mathbf{D}=\{\bar{3}m\}+\{\bar{3}m\}6^{1'}_{111}=6'/m'mm'$.

Completing the determination of the point groups for the CSL dichromatic patterns we consider now the $\Sigma=39b$ $[321]/50{\cdot}13°$ rotation; it cannot be reduced to a 180° rotation. The $\Sigma=39b$ dichromatic pattern contains two ordinary symmetry operations, the (trivial) operations of identity and inversion. In order to check the presence of colour-reversing operations we take $\mathbf{D}_{2,1}=\{1, i, 2^1_{100}, s_{100}\}$ and we note that none of the operations 2^1_{100} and s_{100} satisfy the condition $\mathsf{D}'(\lambda)\ \mathsf{R}\mathsf{D}'(\lambda)R\in\mathbf{D}_o$. The same holds for the subgroups $\mathbf{D}_{2,2}=\{1, i, 2^1_{010}, s_{010}\}$ and $\mathbf{D}_{2,3}=\{1, i, 2^1_{001}, s_{001}\}$. The point group of the $\Sigma=39b$ dichromatic pattern has, therefore, no colour-reversing operations and, hence, $\mathbf{D}=\bar{1}$.

5. Determination of the periodicity of CS lattices

The three-dimensional translation symmetry of a CS lattice can be computed analytically by using (1). However, in the present study an alternative method was used allowing the calculation of three non-coplanar translation vectors $\mathbf{t}_i\in\mathbf{T}(p)$ $(i=1,2,3)$ such that each vector in $\mathbf{T}(p)$ can be written as a linear combination with integral coefficients of $\mathbf{t}_i$. The vectors $\mathbf{t}_i$ $(i=1,2,3)$ form a basis for the group $\mathbf{T}(p)$ and they are expressed in the coordinate system of the white lattice by $\mathbf{t}_i=x_{1i}\mathbf{u}_1+x_{2i}\mathbf{u}_2+x_{3i}\mathbf{u}_3$, where $\mathbf{u}_i$ $(i=1,2,3)$ are the basis vectors of the white coordi-

* We note that Vlachavas (1984) has considered R as the vector transformation relating the black and the white lattices. In the present paper R is taken as a coordinate transformation.

† This does not hold, of course, for the ordinary symmetry elements of identity and inversion, which are not associated with a specific direction in the point group. As was explained above these elements are invariant for any CSL misorientation.

nate system. Thus, the axial representation of the basis of a CS lattice is described by the 3×3 matrix

$$\mathsf{B}=\begin{bmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ x_{31} & x_{32} & x_{33} \end{bmatrix} \equiv [\mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_3],$$

which is called a basis matrix. We have chosen to describe the translational symmetry of CS lattices by the (reduced) Niggli unit cell (Niggli, 1928; *International Tables for Crystallography*, 1983).

The calculation of the basis matrices specifying the Niggli cells of the CS lattices considered in this paper was carried out by a two-stage algorithm. In the first stage we applied the elementary number-theoretical method of Grimmer, Bollmann & Warrington (1974) for calculating the axial representation of an arbitrarily chosen primitive unit cell of a CSL. The corresponding basis matrices for CS lattices in primitive, body-centred and face-centred cubic lattices are denoted by B_p, B_b and B_f, respectively.

The column vectors of matrices B_p, B_b and B_f thus obtained define arbitrary primitive unit cells, which may not be the most cube-like cells, and their vectors may not acquire the shortest length. In the second stage of the algorithm, we convert the unit cell described by B_p, B_b or B_f into the Niggli cell by applying the procedure given by Křivý & Gruber (1976). Also, for each step of the procedure we generate a 3×3 transformation matrix describing the new axial vectors in terms of the old ones so that the overall transformation matrix M and the final basis matrices MB_p, MB_b or MB_f can be printed out when the reduction procedure is complete.

6. Bravais lattices of CSL's

The basis matrices expressing the Niggli unit cells of the CS lattices, obtained by the misorientations listed in Table 1, were calculated by applying the algorithm of the previous section. In these computations the low-index descriptions of the CSL misorientations were used because, as will be discussed in the following, these axis/angle pairs are the most suitable for classifying the symmetry of CSL dichromatic patterns. Tables 2, 3 and 4 list the basis matrices for the CS lattices in primitive cubic (p.c.), face-centred cubic (f.c.c.) and body-centred cubic (b.c.c.) lattices, respectively. The first two columns in these tables give, for each CSL misorientation, the Σ value and the basis matrix $[\mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_3]$ of the Niggli unit cell of the corresponding CS lattice.

The significance in describing the CSL translational periodicity by the Niggli unit cell is not only in its uniqueness, but also in the possibility that it can be used for determining the Bravais type of the CS lattices (Azároff & Buerger, 1958; *International Tables for Crystallography*, 1983). This allows us to establish the metric symmetry of the CS lattices and to calculate the basis matrices $[\boldsymbol{\tau}_1, \boldsymbol{\tau}_2, \boldsymbol{\tau}_3]$ of the conventional unit cells from the primitive triples $[\mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_3]$. The basis matrices $[\boldsymbol{\tau}_1, \boldsymbol{\tau}_2, \boldsymbol{\tau}_3]$ and their Bravais types are tabulated in the last two columns of Tables 2, 3 and 4. The Bravais types are given according to the list:

hP: primitive hexagonal
tP: primitive tetragonal
tI: body-centred tetragonal
hR: rhombohedral hexagonal
oP: primitive orthorhombic
oC: side-centred orthorhombic
oI: body-centred orthorhombic
oF: face-centred orthorhombic
mP: primitive monoclinic
mC: side-centred monoclinic.

The axial representations of the conventional cells are expressed according to the following conventions. In the case of rhombohedral cells, the matrices $[\boldsymbol{\tau}_1, \boldsymbol{\tau}_2, \boldsymbol{\tau}_3]$ are referred to the hexagonal axes. For unit cells in the tetragonal, hexagonal and trigonal systems the relations between the cell dimensions are $|\boldsymbol{\tau}_1| = |\boldsymbol{\tau}_2| \neq |\boldsymbol{\tau}_3|$. In the orthorhombic system the axes of primitive, body-centred and face-centred cells obey the condition $|\boldsymbol{\tau}_1| < |\boldsymbol{\tau}_2| < |\boldsymbol{\tau}_3|$. The side-centred orthorhombic lattice is taken C-centred. In the monoclinic system $\boldsymbol{\tau}_2$ is taken as the unique axis and $\boldsymbol{\tau}_1$, $\boldsymbol{\tau}_3$ are chosen coincident with the shortest two translations perpendicular to $\boldsymbol{\tau}_2$; the angle between $\boldsymbol{\tau}_1$ and $\boldsymbol{\tau}_3$ is taken non acute. The side-centred monoclinic lattice is taken as C-centred.

It should be emphasized that the symmetry determined by means of the Niggli unit cell is the metric symmetry of the CS lattice and it may be the same as or higher than the true symmetry of the CSL dichromatic pattern. This situation is demonstrated by the following examples. Firstly, consider the CSL dichromatic pattern obtained by the misorientation $\Sigma = 21a$ [111]/21·79°; its Bravais lattice is hexagonal and, accordingly, this pattern may contain either a sixfold (high symmetry) or a threefold (low symmetry) rotational axis. However, the high-symmetry case is not consistent with the particular CSL misorientation relationship that is associated with the dichromatic point group $\bar{3}m'$ (§ 4). This becomes apparent by the following considerations. Since the white and black lattices do not contain a sixfold (ordinary) axis, the high-symmetry case should correspond to sixfold colour-reversing rotational symmetry. But the rotation axis is parallel to the direction [111] of the white (and black) lattice, that is, coincident with a threefold ordinary axis and, consequently, in order to have sixfold colour-reversing rotational symmetry, the rotation angle should be equal to 60° (Vlachavas, 1984; see also § 4). This is not the case for the considered example; none of the 24 symmetry-equivalent descriptions of the $\Sigma = 21a$

Table 2. *Basis matrices of the reduced,* $[\mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_3]$, *and the conventional,* $[\boldsymbol{\tau}_1, \boldsymbol{\tau}_2, \boldsymbol{\tau}_3]$, *unit cells of CS lattices* ($\Sigma < 50$) *formed by two primitive cubic lattices*

Σ	$[\mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_3]$			$[\boldsymbol{\tau}_1, \boldsymbol{\tau}_2, \boldsymbol{\tau}_3]$			Symmetry of CSL
3	1	0	1	1	0	1	*hP*
	−1	1	1	−1	1	1	
	0	−1	1	0	−1	1	
5	1	0	0	0	0	1	*tP*
	0	1	−2	1	−2	0	
	0	2	1	2	1	0	
7	1	0	−2	−1	−2	1	*hR*
	1	1	0	3	−1	1	
	1	−2	1	−2	3	1	
9	1	0	2	1	2	−1	*oC*
	1	−1	−2	1	−2	1	
	0	2	−1	0	−1	−4	
11	1	−2	1	1	1	3	*oC*
	1	1	−1	1	−1	−3	
	0	1	3	0	3	−2	
13*a*	1	0	0	0	0	1	*tP*
	0	2	−3	2	−3	0	
	0	3	2	3	2	0	
13*b*	1	−2	−1	−1	−3	1	*hR*
	1	2	−2	4	−1	1	
	1	−1	2	−3	4	1	
15	2	−1	1	−1	−1	2	*oC*
	1	2	−2	2	2	1	
	0	1	2	−5	1	0	
17*a*	1	0	0	0	0	1	*tP*
	0	4	1	4	−1	0	
	0	1	−4	1	4	0	
17*b*	1	−2	2	1	2	3	*oC*
	1	1	−2	1	−2	−3	
	0	2	3	0	3	−4	
19*a*	1	0	3	1	3	−1	*oC*
	1	−1	−3	1	−3	1	
	0	3	−1	0	−1	−6	
19*b*	1	−3	2	−5	2	1	*hR*
	1	0	−3	3	−5	1	
	1	2	0	2	3	1	
21*a*	1	−1	3	−1	3	1	*hP*
	1	−2	−1	−2	−1	1	
	1	3	−2	3	−2	1	
21*b*	2	0	−1	−2	1	2	*oC*
	1	−2	2	1	−2	3	
	0	−1	−4	1	4	1	
23	2	2	1	−1	3	2	*mC*
	1	−3	0	0	−6	1	
	0	−1	−3	3	1	0	
25*a*	1	0	0	0	0	1	*tP*
	0	3	−4	3	−4	0	
	0	4	3	4	3	0	
25*b*	2	1	−1	2	−1	4	*mC*
	1	2	3	1	−2	−5	
	1	−2	2	1	2	−3	
27*a*	1	−1	−3	1	5	−1	*oC*
	1	1	2	1	−5	1	
	0	−5	1	0	−2	−5	
27*b*	2	1	−2	−3	−1	1	*mC*
	1	−3	2	2	2	−3	
	0	−1	−3	1	−7	−1	
29*a*	1	0	0	0	0	1	*tP*
	0	5	−2	5	−2	0	
	0	2	5	2	5	0	
29*b*	2	−1	2	2	−1	2	*mP*
	1	1	−4	1	1	−4	
	0	2	3	0	2	3	
31*a*	1	1	−4	−1	−5	1	*hR*
	1	2	1	6	−1	1	
	1	−4	2	−5	6	1	
31*b*	2	0	−1	2	2	1	*mC*
	1	4	1	1	−7	−1	
	1	−1	3	1	3	−3	
33*a*	1	0	4	1	4	−1	*oC*
	1	−1	−4	1	−4	1	
	0	4	−1	0	−1	−8	

Table 2 (*cont.*)

Σ	$[\mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_3]$			$[\boldsymbol{\tau}_1, \boldsymbol{\tau}_2, \boldsymbol{\tau}_3]$			Symmetry of CSL
33*b*	2	1	1	2	1	−4	*oC*
	1	−4	1	1	1	7	
	1	−1	−3	1	−3	1	
33*c*	1	−2	−3	1	5	−2	*oC*
	1	2	2	1	−5	2	
	0	−5	2	0	−4	−5	
35*a*	2	1	1	−3	1	−1	*oC*
	1	−5	−1	0	2	5	
	1	3	−2	1	3	−3	
35*b*	2	1	−2	−1	−3	−2	*oC*
	1	−2	4	2	6	−1	
	0	−3	−1	3	−5	0	
37*a*	1	0	0	0	0	1	*tP*
	0	6	1	6	−1	0	
	0	1	−6	1	6	0	
37*b*	2	−1	−2	−3	1	2	*mC*
	2	3	1	−1	−3	2	
	1	0	4	8	0	1	
37*c*	1	−4	3	−7	3	1	*hR*
	1	0	−4	4	−7	1	
	1	3	0	3	4	1	
39*a*	1	3	1	3	1	1	*hP*
	1	−4	3	−4	3	1	
	1	1	−4	1	−4	1	
39*b*	0	3	−2	−5	−1	0	*mC*
	0	2	3	1	−5	0	
	3	1	1	0	−2	3	
41*a*	1	0	0	0	0	1	*tP*
	0	4	−5	4	−5	0	
	0	5	4	5	4	0	
41*b*	2	−2	1	2	−2	1	*mP*
	1	2	−2	1	2	−2	
	0	1	6	0	1	6	
41*c*	1	−4	1	1	−3	−4	*oC*
	1	4	−2	1	3	4	
	0	3	4	0	−8	3	
43*a*	1	4	−3	6	−7	1	*hR*
	1	−2	4	1	6	1	
	1	−3	−2	−7	1	1	
43*b*	2	−1	0	1	1	2	*mC*
	1	4	1	−2	−4	1	
	0	1	5	9	−1	0	
43*c*	1	−3	−3	1	5	−3	*oC*
	1	3	2	1	−5	3	
	0	−5	3	0	−6	−5	
45*a*	2	−4	1	3	5	−1	*mC*
	2	1	−3	−1	−1	3	
	1	3	1	2	−8	−1	
45*b*	2	−2	−1	2	−2	−1	*oP*
	1	4	2	1	4	2	
	0	−5	2	0	−5	2	
45*c*	2	−1	−4	1	−7	1	*mC*
	2	1	1	3	5	−1	
	1	−3	3	−2	4	3	
47*a*	2	1	−3	−3	−3	1	*mC*
	1	−3	4	2	6	−3	
	0	−3	−2	3	−7	−3	
47*b*	3	0	1	3	3	−1	*mC*
	1	5	1	1	−9	−1	
	0	−1	3	0	2	−3	
49*a*	1	−1	4	−5	8	1	*hR*
	1	−4	−1	−3	−5	1	
	1	4	−4	8	−3	1	
49*b*	2	−1	−1	2	4	1	*mC*
	1	5	0	1	−9	0	
	1	0	4	1	1	−4	
49*c*	2	0	−3	2	0	−3	*mP*
	1	−1	6	1	−1	6	
	0	−3	−2	0	−3	−2	

Table 3. *Basis matrices of the reduced,* $[\mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_3]$, *and the conventional,* $[\boldsymbol{\tau}_1, \boldsymbol{\tau}_2, \boldsymbol{\tau}_3]$, *unit cells of CS lattices* ($\Sigma < 50$) *formed by two face-centred cubic lattices*

Σ	$[\mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_3]$			$[\boldsymbol{\tau}_1, \boldsymbol{\tau}_2, \boldsymbol{\tau}_3]$			Symmetry of CSL
3	−1/2	0	1	−1/2	0	1	*hP*
	1/2	−1/2	1	1/2	−1/2	1	
	0	1/2	1	0	1/2	1	
5	1	1/2	1/2	0	0	1	*tI*
	0	1/2	−1	3/2	−1/2	0	
	0	1	1/2	1/2	3/2	0	
7	−1/2	−1	1/2	1/2	1	1	*hR*
	−1	1/2	−1/2	−3/2	1/2	1	
	1/2	−1/2	−1	1	−3/2	1	
9	1/2	−1	−1/2	1/2	2	−1/2	*oI*
	1/2	3/2	1	1/2	−2	1/2	
	0	−1/2	3/2	0	−1	−2	
11	1/2	−1	−1	1/2	3/2	−1	*oC*
	1/2	1	1/2	1/2	−3/2	1	
	0	−3	1/2	0	−1	−3	
13*a*	1	1/2	1/2	0	0	1	*tI*
	0	−1	3/2	5/2	−1/2	0	
	0	−3/2	−1	1/2	5/2	0	
13*b*	0	3/2	−1/2	1/2	3/2	1	*hR*
	−1/2	0	3/2	−2	1/2	1	
	3/2	−1/2	0	3/2	−2	1	
15	1/2	3/2	−1/2	−1/2	−2	1/2	*oI*
	−1	−1/2	−3/2	1	−1	−1	
	−1/2	1	1	1/2	0	5/2	
17*a*	1	1/2	1/2	0	0	1	*tI*
	0	1/2	2	3/2	−5/2	0	
	0	−2	1/2	5/2	3/2	0	
17*b*	1/2	0	−3/2	1/2	2	3/2	*oI*
	1/2	1/2	2	1/2	−2	−3/2	
	0	−5/2	−1/2	0	3	−2	
19*a*	1/2	−3	0	1/2	−1/2	−3	*oC*
	1/2	3	−1/2	1/2	1/2	3	
	0	1	3/2	0	−3	1	
19*b*	1	−3/2	−1/2	−5/2	1	1	*hR*
	1	1	−3/2	3/2	−5/2	1	
	1	−1/2	1	1	3/2	1	
21*a*	1	1/2	−3/2	1/2	−3/2	1	*hP*
	1	1	1/2	1	1/2	1	
	1	−3/2	1	−3/2	1	1	
21*b*	−1	1	−1/2	1	−1	−1	*oI*
	1/2	3/2	0	−1/2	−3/2	2	
	1/2	1/2	−5/2	−1/2	−1/2	−4	
23	−1/2	−1	−2	−1/2	3/2	2	*mC*
	0	3/2	−1	0	−3	1	
	3/2	1/2	0	3/2	1/2	0	
25*a*	1	1/2	1/2	0	0	1	*tI*
	0	3/2	−2	7/2	−1/2	0	
	0	2	3/2	1/2	7/2	0	
25*b*	1	−1/2	0	1	2	0	*mC*
	1/2	3/2	−3/2	1/2	−5/2	3/2	
	1/2	1	5/2	1/2	−3/2	−5/2	
27*a*	1/2	−3/2	1	1/2	1	5/2	*oC*
	1/2	1	−1	1/2	−1	−5/2	
	0	1/2	5	0	5	−1	
27*b*	−3/2	1/2	1/2	1/2	3/2	−1/2	*mC*
	1	1/2	2	2	−1	1	
	1/2	2	1/2	1/2	−1/2	−7/2	
29*a*	1	1/2	1/2	0	0	1	*tI*
	0	1	5/2	3/2	−7/2	0	
	0	−5/2	1	7/2	3/2	0	
29*b*	1/2	2	2	2	−2	−1/2	*mC*
	−1/2	1	−3/2	1	4	1/2	
	−1	0	3/2	0	−3	1	
31*a*	1	−3/2	−1	−1/2	−5/2	1	*hR*
	1	3/2	−3/2	3	−1/2	1	
	1	−1	3/2	−5/2	3	1	
31*b*	1	−3/2	−1/2	−1	−2	1	*mC*
	1/2	2	−3/2	7/2	1/2	1/2	
	1/2	1/2	2	−3/2	5/2	1/2	
33*a*	1/2	−2	−3/2	1/2	4	−1/2	*oI*
	1/2	5/2	2	1/2	−4	1/2	
	0	−3/2	5/2	0	−1	−4	
33*b*	1	−1	1/2	1	−2	−1	oC
	1/2	−1	−2	1/2	7/2	−1	
	1/2	3	−1/2	1/2	1/2	3	
33*c*	1/2	0	5/2	1/2	5/2	−2	*oI*
	1/2	1/2	−2	1/2	−5/2	2	
	0	7/2	3/2	0	−2	−5	
35*a*	1	1/2	−1	3/2	−1/2	−1	*oC*
	1/2	−1/2	5	0	−1	5	
	1/2	−1	−3	−1/2	−3/2	−3	
35*b*	1/2	−2	0	−1/2	2	−3/2	*oI*
	−1	−1	5/2	1	1	3	
	−3/2	0	−1/2	3/2	0	−5/2	
37*a*	1	1/2	1/2	0	0	1	*tI*
	0	1/2	3	5/2	−7/2	0	
	0	−3	1/2	7/2	5/2	0	
37*b*	1/2	−2	−1/2	5/2	−1/2	−3/2	*mC*
	−3/2	−1/2	0	1/2	3/2	−1/2	
	0	3/2	−5/2	1	0	4	
37*c*	1	−2	−1/2	−7/2	3/2	1	*hR*
	1	3/2	−2	2	−7/2	1	
	1	−1/2	3/2	3/2	2	1	
39*a*	1	−3/2	−1/2	−3/2	−1/2	1	*hP*
	1	2	−3/2	2	−3/2	1	
	1	−1/2	2	−1/2	2	1	
39*b*	3/2	−1	0	1/2	5/2	0	*mC*
	1	3/2	0	5/2	−1/2	0	
	1/2	1/2	3	1	0	−3	
41*a*	1	1/2	1/2	0	0	1	*tI*
	0	−2	5/2	9/2	−1/2	0	
	0	−5/2	−2	1/2	9/2	0	
41*b*	0	−2	1/2	2	−1	−2	*mC*
	−3/2	1/2	3/2	1	2	1/2	
	−1/2	1/2	−3	0	−6	1/2	
41*c*	1/2	3	3/2	1/2	−3/2	−4	*oI*
	1/2	−5/2	−1	1/2	3/2	4	
	0	1/2	−7/2	0	−4	3	
43*a*	1	1/2	−5/2	3	−7/2	1	*hR*
	1	1	1/2	1/2	3	1	
	1	−5/2	1	−7/2	1/2	1	
43*b*	1/2	−2	0	1/2	1/2	2	*mC*
	−2	−1	−1/2	−1	−2	1	
	−1/2	0	−5/2	9/2	−1/2	0	
43*c*	1/2	−3/2	3	1/2	3	5/2	oC
	1/2	1	−3	1/2	−3	−5/2	
	0	3/2	5	0	5	−3	
45*a*	−3/2	−2	1/2	−3/2	5/2	−1/2	*mC*
	1/2	1/2	5/2	1/2	−1/2	−5/2	
	−1	3/2	0	−1	−4	0	
45*b*	1/2	3/2	−2	2	2	1	*oF*
	3/2	−1/2	3/2	1	−4	−2	
	1	−1	−5/2	0	5	−2	
45*c*	1/2	2	−3/2	1/2	−7/2	3/2	*mC*
	3/2	−1/2	−1/2	3/2	5/2	1/2	
	−1	−3/2	−2	−1	2	2	
47*a*	2	−1	−3/2	1/2	3/2	3/2	*mC*
	1	1/2	1	2	−3	−1	
	0	−5/2	3/2	3/2	7/2	−3/2	
47*b*	3/2	1/2	0	3/2	−1/2	3/2	*mC*
	1/2	−1/2	5/2	1/2	1/2	−9/2	
	0	−3	−1/2	0	3	1	
49*a*	1	−5/2	3/2	−5/2	4	1	*hR*
	1	0	−5/2	−3/2	−5/2	1	
	1	3/2	0	4	−3/2	1	
49*b*	1	2	−1/2	1	−2	2	*mC*
	1/2	1/2	5/2	1/2	−1/2	−9/2	
	1/2	−7/2	0	1/2	7/2	1/2	
49*c*	0	2	−1/2	2	3	0	*mC*
	1/2	1	7/2	1	−6	−1/2	
	3/2	0	−1	0	2	−3/2	

Table 4. *Basis matrices of the reduced,* $[\mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_3]$, *and the conventional,* $[\boldsymbol{\tau}_1, \boldsymbol{\tau}_2, \boldsymbol{\tau}_3]$, *unit cells of CS lattices* ($\Sigma<50$) *formed by two body-centred cubic lattices*

Σ	$[\mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_3]$			$[\boldsymbol{\tau}_1, \boldsymbol{\tau}_2, \boldsymbol{\tau}_3]$			Symmetry of CSL
3	1/2	1	0	1	0	1/2	*hP*
	1/2	−1	1	−1	1	1/2	
	1/2	0	−1	0	−1	1/2	
5	1	1/2	1/2	0	0	1	*tI*
	0	3/2	−1/2	1	−2	0	
	0	1/2	3/2	2	1	0	
7	1/2	3/2	−3/2	2	−3	1/2	*hR*
	1/2	−1/2	3/2	1	2	1/2	
	1/2	−3/2	−1/2	−3	1	1/2	
9	1	3/2	0	1	2	−1	*oF*
	1	−1/2	1	1	−2	1	
	0	−1/2	−2	0	−1	−4	
11	1	−1/2	−2	1	3	−1/2	*oC*
	1	1/2	1	1	−3	1/2	
	0	−3/2	1	0	−2	−3/2	
13*a*	1	1/2	1/2	0	0	1	*tI*
	0	−5/2	1/2	2	−3	0	
	0	−1/2	−5/2	3	2	0	
13*b*	1/2	−5/2	3/2	−4	1	1/2	*hR*
	1/2	1/2	−5/2	3	−4	1/2	
	1/2	3/2	1/2	1	3	1/2	
15	1/2	3/2	−3/2	2	1	1	*oF*
	3/2	−1/2	1/2	1	−2	−2	
	1/2	−1/2	−5/2	0	5	−1	
17*a*	1	1/2	1/2	0	0	1	*tI*
	0	5/2	3/2	4	−1	0	
	0	−3/2	5/2	1	4	0	
17*b*	1	3/2	2	1	2	3	*oF*
	1	−1/2	−1	1	−2	−3	
	0	3/2	−2	0	3	−4	
19*a*	1	−3/2	0	1	−1	−3/2	*oC*
	1	3/2	−1	1	1	3/2	
	0	1/2	3	0	−6	1/2	
19*b*	1/2	−1/2	5/2	−3	5	1/2	*hR*
	1/2	−5/2	−1/2	−2	−3	1/2	
	1/2	5/2	−5/2	5	−2	1/2	
21*a*	1/2	1	−3	1	−3	1/2	*hP*
	1/2	2	1	2	1	1/2	
	1/2	−3	2	−3	2	1/2	
21*b*	0	2	−1/2	−2	−2	1	*oF*
	−2	1	−1/2	1	−3	−2	
	−1	0	5/2	1	−1	4	
23	1/2	1/2	3/2	2	−3	−3/2	*mC*
	1/2	−7/2	1/2	1	6	−1/2	
	3/2	1/2	−3/2	0	−1	3/2	
25*a*	1	1/2	1/2	0	0	1	*tI*
	0	7/2	−1/2	3	−4	0	
	0	1/2	7/2	4	3	0	
25*b*	−1/2	−3/2	−1	2	−4	−3/2	*mC*
	1/2	−3/2	3	1	5	−3/2	
	−3/2	1/2	2	1	3	1/2	
27*a*	1	−3	1/2	1	1/2	5	*oC*
	1	2	−1/2	1	−1/2	−5	
	0	1	5/2	0	5/2	−2	
27*b*	1/2	−2	−3/2	2	1/2	−1	*mC*
	−3/2	−1	1/2	1	−3/2	2	
	−1/2	0	−7/2	0	−1/2	−7	
29*a*	1	1/2	1/2	0	0	1	*tI*
	0	7/2	3/2	5	−2	0	
	0	−3/2	7/2	2	5	0	
29*b*	2	1	−1/2	−2	−1	2	*mC*
	1	−1	3/2	4	1	1	
	0	−2	−5/2	−3	2	0	
31*a*	1/2	7/2	−5/2	5	−6	1	*hR*
	1/2	−3/2	7/2	1	5	1	
	1/2	−5/2	−3/2	−6	1	1	
31*b*	−1/2	2	0	2	2	1/2	*mC*
	1/2	1	4	1	−7	−1/2	
	3/2	1	−1	1	3	−3/2	
33*a*	1	5/2	0	1	4	−1	*oF*
	1	−3/2	1	1	−4	1	
	0	−1/2	−4	0	−1	−8	

Table 4 (*cont.*)

Σ	$[\mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_3]$			$[\boldsymbol{\tau}_1, \boldsymbol{\tau}_2, \boldsymbol{\tau}_3]$			Symmetry of CSL
33*b*	1/2	2	1	2	1/2	−4	*oC*
	1/2	1	−4	1	1/2	7	
	−3/2	1	−1	1	−3/2	1	
33*c*	1	3	−1/2	1	5	−2	*oF*
	1	−2	3/2	1	−5	2	
	0	−2	−5/2	0	4	−5	
35*a*	2	1	−1/2	3	−1	−1/2	*oC*
	1	−1	5/2	0	−2	5/2	
	1	−2	−3/2	−1	−3	−3/2	
35*b*	3/2	1/2	1/2	2	−3	−1	*oF*
	−1/2	3/2	−7/2	1	6	2	
	−3/2	3/2	5/2	0	−5	3	
37*a*	1	1/2	1/2	0	0	1	*tI*
	0	7/2	5/2	6	−1	0	
	0	−5/2	7/2	1	6	0	
37*b*	3/2	1/2	−5/2	2	−1/2	3	*mC*
	−1/2	5/2	−3/2	2	−5/2	1	
	1/2	1/2	7/2	1	−1/2	−8	
37*c*	1/2	−1/2	7/2	−4	7	1	*hR*
	1/2	−7/2	−1/2	−3	−4	1	
	1/2	7/2	−7/2	7	−3	1	
39*a*	1/2	−3	−1	−3	−1	1/2	*hP*
	1/2	4	−3	4	−3	1/2	
	1/2	−1	4	−1	4	1/2	
39*b*	−1/2	−5/2	5/2	0	5	−1/2	*mC*
	−5/2	1/2	−1/2	0	−1	−5/2	
	1/2	−3/2	−3/2	−3	0	1/2	
41*a*	1	1/2	1/2	0	0	1	*tI*
	0	−9/2	1/2	4	−5	0	
	0	−1/2	−9/2	5	4	0	
41*b*	2	−1/2	−2	0	1	2	*mC*
	1	−1/2	2	3	−2	−2	
	0	−7/2	−1	1	6	−1	
41*c*	1	−1	−3/2	1	−3	−4	*oF*
	1	2	5/2	1	3	4	
	0	−4	3/2	0	−8	3	
43*a*	1/2	5/2	3/2	7	−1	1/2	*hR*
	1/2	−9/2	5/2	−6	7	1/2	
	1/2	3/2	−9/2	−1	−6	1/2	
43*b*	−3/2	−2	−1/2	2	−3/2	1	*mC*
	3/2	−1	−3/2	1	3/2	−2	
	1/2	0	9/2	0	1/2	9	
43*c*	1	−3	3/2	1	3/2	5	*oC*
	1	2	−3/2	1	−3/2	−5	
	0	3	5/2	0	5/2	−6	
45*a*	1/2	−5/2	7/2	2	5	−5/2	*mC*
	−3/2	−1/2	1/2	2	−1	−1/2	
	1/2	−3/2	−7/2	1	−8	−3/2	
45*b*	2	−1	1/2	2	−2	−1	*oI*
	1	2	−7/2	1	4	2	
	0	2	3/2	0	−5	2	
45*c*	1/2	3/2	−9/2	2	−3/2	7	*mC*
	−1/2	5/2	3/2	2	−5/2	−5	
	3/2	−1/2	3/2	1	1/2	−4	
47*a*	1/2	−2	−5/2	2	1/2	−3	*mC*
	−3/2	−1	5/2	1	−3/2	6	
	−3/2	0	−7/2	0	−3/2	−7	
47*b*	1	0	5/2	3	−3	−5/2	*mC*
	1	−5	1/2	1	9	−1/2	
	3	1	−3/2	0	−2	3/2	
49*a*	1/2	7/2	1/2	3	5	1/2	*hR*
	1/2	−9/2	7/2	−8	3	1/2	
	1/2	1/2	−9/2	5	−8	1/2	
49*b*	−3/2	−2	1	2	−3/2	4	*mC*
	−1/2	−1	−5	1	−1/2	−9	
	3/2	−1	0	1	3/2	1	
49*c*	2	0	3/2	3	0	2	*mC*
	1	1	−5/2	−6	−1	1	
	0	3	5/2	2	−3	0	

misorientation corresponds to a 60° rotation along a ⟨111⟩ direction (Warrington & Bufalini, 1971).

In the second example we consider the dichromatic patterns for $\Sigma = 15$ [210]/48·19°. The translational symmetry of these patterns is described by a side-centred, body-centred or face-centred orthorhombic lattice depending on whether the white (and black) lattice is p.c., f.c.c. or b.c.c., respectively. The true symmetry of the patterns must, however, be lower since, as mentioned in § 4, the point group of the particular CSL misorientation is $2'/m'$. This suggests that the orthogonality of the axes in the non-primitive unit cells of these patterns must be regarded as accidental. In fact, such pseudo-orthorhombic symmetry occurs for $\Sigma = 15$, $21b$, $33b$, $35a$, $35b$ and $45b$. A similar situation is encountered for the $\Sigma = 39b$ CSL dichromatic pattern in which the periodicity is described by a side-centred monoclinic lattice and its point group is $\bar{1}$. Again, the pseudo-monoclinic symmetry of this pattern is due to accidentally special values of the interaxial angles.

It is clear that, in cases like the ones just mentioned, only the metric symmetry of CS lattices fails to reveal the true symmetry of the corresponding CSL dichromatic patterns.* For the unambiguous determination of their symmetry it is necessary, as explained in § 3, to combine the dichromatic point symmetry with the three-dimensional translational symmetry of the associated CS lattice.

7. Space symmetry of CSL dichromatic patterns

The space groups of the CSL dichromatic patterns formed by two p.c., b.c.c. or f.c.c. lattices are given in Table 5. As can be seen, the considered dichromatic patterns belong to one of the following systems: hexagonal, tetragonal, trigonal orthorhombic, monoclinic and triclinic. Furthermore, we note that there is only one dichromatic pattern of hexagonal symmetry and it corresponds to $\Sigma = 3$ [111]/60° (or symmetry equivalent) misorientation. Also, only one dichromatic pattern ($\Sigma = 39b$) of triclinic symmetry exists for CSL rotations with $\Sigma < 50$.† The remaining CSL misorientations in the cubic system are classified, on the grounds of their low-index descriptions, into four distinct categories. The first three categories contain rotations about [100], [110] and [111], respectively. In the fourth category we have CSL misorientations whose low-index descriptions correspond to rotations along [210], [211], [221], [310].

The patterns obtained by rotations about the [100] axis have tetragonal symmetry . For the p.c. case the

Table 5. *Space groups of CSL dichromatic patterns ($\Sigma < 50$) formed by two primitive cubic, body-centred cubic or face-centred cubic lattices*

Σ	p.c.	b.c.c.	f.c.c.
3	$P6'/m'mm'$	$P6'/m'mm'$	$P6'/m'mm'$
5	$P4/mm'm'$	$I4/mm'm'$	$I4/mm'm'$
7	$R\bar{3}m'$	$R\bar{3}m'$	$R\bar{3}m'$
9	$Cmm'm'$	$Fm'm'm$	$Im'm'm$
11	$Cmm'm'$	$Cmm'm'$	$Cmm'm'$
13a	$P4/mm'm'$	$I4/mm'm'$	$I4/mm'm'$
13b	$R\bar{3}m'$	$R\bar{3}m'$	$R\bar{3}m'$
15	$C2'/m'$	$C2'/m'$	$C2'/m'$
17a	$P4/mm'm'$	$I4/mm'm'$	$I4/mm'm'$
17b	$Cmm'm'$	$Fm'm'm$	$Im'm'm$
19a	$Cmm'm'$	$Cmm'm'$	$Cmm'm'$
19b	$R\bar{3}m'$	$R\bar{3}m'$	$R\bar{3}m'$
21a	$P\bar{3}1m'$	$P\bar{3}1m'$	$P\bar{3}1m'$
21b	$C2'/m'$	$C2'/m'$	$C2'/m'$
23	$C2'/m'$	$C2'/m'$	$C2'/m'$
25a	$P4/mm'm'$	$I4/mm'm'$	$I4/mm'm'$
25b	$C2'/m'$	$C2'/m'$	$C2'/m'$
27a	$Cmm'm'$	$Cmm'm'$	$Cmm'm'$
27b	$C2'/m'$	$C2'/m'$	$C2'/m'$
29a	$P4/mm'm'$	$I4/mm'm'$	$I4/mm'm'$
29b	$P2'/m'$	$C2'/m'$	$C2'/m'$
31a	$R\bar{3}m'$	$R\bar{3}m'$	$R\bar{3}m'$
31b	$C2'/m'$	$C2'/m'$	$C2'/m'$
33a	$Cmm'm'$	$Fm'm'm$	$Im'm'm$
33b	$C2'/m'$	$C2'/m'$	$C2'/m'$
33c	$Cmm'm'$	$Fm'm'm$	$Im'm'm$
35a	$C2'/m'$	$C2'/m'$	$C2'/m'$
35b	$C2'/m'$	$C2'/m'$	$C2'/m'$
37a	$P4/mm'm'$	$I4/mm'm'$	$I4/mm'm'$
37b	$C2'/m'$	$C2'/m'$	$C2'/m'$
37c	$R\bar{3}m'$	$R\bar{3}m'$	$R\bar{3}m'$
39a	$P\bar{3}1m'$	$P\bar{3}1m'$	$P\bar{3}1m'$
39b	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$
41a	$P4/mm'm'$	$I4/mm'm'$	$I4/mm'm'$
41b	$P2'/m'$	$C2'/m'$	$C2'/m'$
41c	$Cmm'm'$	$Fm'm'm$	$Im'm'm$
43a	$R\bar{3}m'$	$R\bar{3}m'$	$R\bar{3}m'$
43b	$C2'/m'$	$C2'/m'$	$C2'/m'$
43c	$Cmm'm'$	$Cmm'm'$	$Cmm'm'$
45a	$C2'/m'$	$C2'/m'$	$C2'/m'$
45b	$P2'/m'$	$C2'/m'$	$C2'/m'$
45c	$C2'/m'$	$C2'/m'$	$C2'/m'$
47a	$C2'/m'$	$C2'/m'$	$C2'/m'$
47b	$C2'/m'$	$C2'/m'$	$C2'/m'$
49a	$R\bar{3}m'$	$R\bar{3}m'$	$R\bar{3}m'$
49b	$C2'/m'$	$C2'/m'$	$C2'/m'$
49c	$P2'/m'$	$C2'/m'$	$C2'/m'$

unit cell is primitive, its c axis is along [100] and the axial ratio is $c/a = 1/\Sigma^{1/2}$. On the other hand, body-centred unit cells occur for the dichromatic patterns formed by f.c.c. or b.c.c. lattices. The c axis is parallel to [100] and the axial ratio is $c/a = (2/\Sigma)^{1/2}$ for f.c.c. or $c/a = 1/\Sigma^{1/2}$ for b.c.c. lattices.

The CSL rotations about [110] are associated with dichromatic patterns of point symmetry $mm'm'$ in which the two fold ordinary symmetry axis is parallel to [110]. The orthorhombic unit cell has the a axis along the twofold ordinary axis and its length is $2^{1/2}$ for the p.c. and b.c.c. lattices, but $1/2^{1/2}$ for the f.c.c. lattices. The space group of the dichromatic patterns for p.c. lattices is $Cmm'm'$ with axial ratios $a:b:c = 2^{1/2}:2\Sigma^{1/2}:\Sigma^{1/2}$. When the white (and black) lattice is f.c.c., then two types of CSL dichromatic patterns are formed. These two types are distinguished by noting that all the [110] CSL rotations can be alterna-

*The metric symmetry of CS lattices for p.c., b.c.c. or f.c.c. lattices up to $\Sigma = 21$ has recently been determined by Andreyeva (1983). We must, however, point out that the results for b.c.c. and f.c.c. lattices appear in Andreyeva's tables in the wrong order.

†Tabulated values of CSL misorientations (Mykura, 1980) indicate that there are 17 triclinic dichromatic patterns for $\Sigma < 100$.

tively described by a 180° rotation along a $[u_1u_1w_1]$ or $[u_2v_2v_2]$ direction. Then, a body-centred orthorhombic CS lattice is formed when u_1 or v_2 is even (type I) and a base-centred orthorhombic CS lattice when u_1 and v_2 are odd (type II). The axial ratios for both types of orthorhombic lattices are $a:b:c=(1/2)^{1/2}:(\Sigma/2)^{1/2}:\Sigma^{1/2}$. Two types of orthorhombic CSL dichromatic pattern occur again for b.c.c. lattices depending on u_1 or v_2. They are either face-centred (type I; when u_1 or v_2 is even) or base-centred (type II; u_1 and v_2 are equal to an odd number) orthorhombic lattices. The axial ratios are $a:b:c=2^{1/2}:\Sigma^{1/2}:(2\Sigma)^{1/2}$ or $a:b:c=2^{1/2}:(2\Sigma)^{1/2}:(\Sigma/4)^{1/2}$ for F or C lattices, respectively.

The lattices of CSL dichromatic patterns corresponding to [111] rotations are hexagonal or rhombohedral with the principal axis parallel to [111], the length of which is $3^{1/2}$ for the p.c. or f.c.c. lattices but $3^{1/2}/2$ for the b.c.c. lattices. For all p.c., f.c.c. and b.c.c. cases, the space group of the $\Sigma=3$ dichromatic pattern is $P6'/m'mm'$. All the other [111] rotations yield dichromatic patterns of trigonal symmetry. Two types of trigonal space groups are formed depending on whether or not Σ is a multiple of 3. In type I belong dichromatic patterns with $\Sigma=7, 13b, 19b, 31a, 37c, 43a, 49a$ and they have a non-primitive unit cell (rhombohedral cell) with $c/a=(3/2\Sigma)^{1/2}$ for p.c. lattices, $c/a=(3/8\Sigma)^{1/2}$ for b.c.c. lattices or $c/a=(6/\Sigma)^{1/2}$ for f.c.c. lattices. If $\Sigma=3n$, where n is an integer, the dichromatic patterns (for $\Sigma=21a$ and $\Sigma=39a$) possess a primitive hexagonal unit cell with $c/a=(3/2n)^{1/2}$, $(6/n)^{1/2}$, $(3/8n)^{1/2}$ when the white (and black) lattice is p.c., f.c.c. or b.c.c., respectively.

It remains, now, to consider the space groups for the rest of the CSL rotations. With the exception of the $\Sigma=39b$ CSL misorientation, all these rotations yield dichromatic patterns of monoclinic symmetry. In these cases the expression of the axial ratios by general relations is not desirable owing to the large number of different types of unit cells that have to be considered. For instance, in the case of CSL dichromatic patterns with pseudo-orthorhombic symmetry we have to consider three types of unit cells. Type I corresponds to $\Sigma=15$ [210]/48·19° and $\Sigma=35b$ [210]/106·60° and the axial ratios of the associated unit cells are $a:b:c=(2\Sigma/d)^{1/2}:(2\Sigma)^{1/2}:d^{1/2}$, $(\Sigma/2d)^{1/2}:d^{1/2}:(\Sigma/2)^{1/2}$ or $d^{1/2}:(2\Sigma/d)^{1/2}:(2\Sigma)^{1/2}$, where $d=2^2+1=5$, depending on whether the white (and black) lattice is p.c., f.c.c. or b.c.c., respectively. Type II refers to $\Sigma=45b$ [210]/83·62° dichromatic patterns and $a:b:c=d^{1/2}:(\Sigma/d)^{1/2}:\Sigma^{1/2}$, where $d=5$, for all p.c., f.c.c. and b.c.c. cases. The last type of pseudo-orthorhombic dichromatic patterns contains the $\Sigma=21b$ [210]/58·41° and $\Sigma=35a$ [211]/34·05° misorientations. In the case of p.c. or f.c.c. lattices the axial ratios of the unit cells are $a:b:c=(4\Sigma/d)^{1/2}:d^{1/2}:\Sigma^{1/2}$ or $(\Sigma/d)^{1/2}:(d/4)^{1/2}:\Sigma^{1/2}$, respectively, where $d=14$.

8. Conclusions

In the preceding sections a procedure was presented enabling the determination of the symmetry of a CSL dichromatic pattern knowing the rotation axis and rotation angle characterizing it. By using this methodology, the symmetry of a dichromatic pattern formed by two identical cubic lattices was investigated by combining the three-dimensional periodicity of the associated CS lattice with the point-symmetry operations of the motif characterizing the particular dichromatic pattern. This provides a very elegant and concise formulation for treating this subject, especially if antisymmetry (two-coloured symmetry) is used as suggested by Pond & Bollmann (1979).

A dichromatic pattern is considered as a composite formed by the appropriate superposition of a black and a white lattice. This permits us to apply the principle of the symmetry of composites (see *e.g.* Shubnikov & Koptsik, 1977) and to use group-theoretical procedures for determining the point group of a dichromatic pattern. The treatment shows that all dichromatic patterns in the cubic system are centrosymmetric and their possible point groups are $4/mmm'm'$, $6'/m'mm'$, $\bar{3}m'$, $mm'm'$, $2'/m'$, $\bar{1}$.

The periodicity of a CS lattice, on the other hand, was expressed by means of the reduced (Niggli) unit cell. This ensures uniqueness in the description of the three-dimensional translational symmetry of the particular CS lattice. Also, it permits the determination of the corresponding conventional unit cell so that the derivation of the space group of the dichromatic pattern is carried out in a straightforward manner.

The determination of all possible space groups for CSL dichromatic patterns in the cubic system is valuable for several reasons. Firstly, systematic classification in this way enables the grouping of dichromatic patterns into classes and, also, permits any generic relations between dichromatic patterns with the same Σ but formed by two p.c., b.c.c. or f.c.c. lattices to be established. Secondly, it becomes possible to relate uniquely a coordinate pattern to the symmetry elements of a dichromatic pattern, thus ensuring uniqueness of description for its associated bicrystals.

Concluding this paper, we must point out that the symmetry of the dichromatic pattern is uniquely related to the axes of the 180° rotation creating the pattern. This is shown in Fig. 1, which represents the stereographic projection in the reference triangle of the 180° rotation axes of all CSL misorientations in the cubic system with $\Sigma<50$. Each rotation axis is marked by a solid square, open circle, solid triangle and solid circle depending on whether the corresponding dichromatic pattern exhibits tetragonal, orthorhombic, trigonal or monoclinic symmetry, respectively. The $\Sigma=3$ [111]/180° and [211]/180° misorientations, associated with hexagonal symmetry, are shown by crosses. We note that the misorientations of dichromatic patterns with point symmetry $4/mm'm'$ are described by 180° rotations along directions lying on the arc of the circle passing through [100] and [110]. Similarly, the orthorhombic groups $mm'm'$ correspond to directions in the sections [100]-[111] and [110]-[111] of the standard stereographic triangle and the trigonal groups $\bar{3}m'$ to the section [110]-[211].

It is also interesting to mention that the symmetry of the dichromatic pattern defines uniquely the number N of different misorientations that create a given CS lattice. Grimmer (1973) has shown that N is a multiple of 24, *i.e.* $N = 24M$, where M is unambiguously determined by the crystal class of the corresponding dichromatic pattern according to the following table:

M	crystal class of the dichromatic pattern
48	triclinic
24	monoclinic
12	orthorhombic
8	trigonal
6	tetragonal
4	hexagonal.

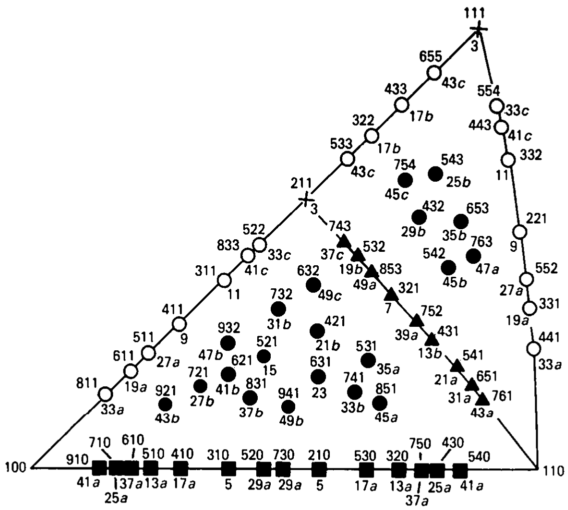

Fig. 1. Stereographic projection in the reference triangle of the 180° rotation axes of CSL misorientations with $\Sigma < 50$ in the cubic system. Rotation axes are represented by solid squares, solid triangles, open circles or solid circles depending on whether the corresponding dichromatic patterns exhibit tetragonal, trigonal, orthorhombic or monoclinic point symmetry, respectively. The $\Sigma = 3$ [111]/180° and [211]/180° CSL misorientations giving rise to dichromatic patterns with hexagonal point symmetry are represented by crosses.

We further note that, if r denotes the order of the point group of the dichromatic pattern, then $Nr =$ constant. This relation is a consequence of the dissymmetrization taking place during the formation of the given dichromatic pattern. In general terms, we have a reduction in the symmetry of the dichromatic pattern in comparison with the symmetry of its parts, *i.e.* the white and black lattices. Then, according to the principle of symmetry conservation (mathematically expressed by the Lagrange theorem), there exist crystallographically equivalent ways of obtaining a given dichromatic pattern and these are interrelated by the symmetry operations of the white (or black) lattice supressed by the formation of the pattern.

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