

in reciprocal-space components; 0, 0, 1 in the case of K_2PtCl_4) lies in the plane of scattering or perpendicular to it. The angles and coordinate system used here are defined as for the Enraf-Nonius CAD-4 diffractometer; this coordinate system is not the same as that used in the main text. First calculate Eulerian setting angles ϕ and χ for $\psi = 0$. For these angles \mathbf{h} is along the y axis and the direction of \mathbf{d} is $\mathbf{s} = \mathbf{XZRd}$, where \mathbf{R} is the reciprocal-space orientation matrix and

$$\mathbf{s} = \begin{pmatrix} s_1 \\ s_2 \\ s_3 \end{pmatrix}, \mathbf{X}(\chi) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \chi & \sin \chi \\ 0 & -\sin \chi & \cos \chi \end{pmatrix},$$

$$\mathbf{Z}(\phi) = \begin{pmatrix} \cos \phi & \sin \phi & 0 \\ -\sin \phi & \cos \phi & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

An azimuthal rotation about the y axis by an angle ψ ,

$$\psi = \tan^{-1}(s_3/s_1),$$

places \mathbf{d} in the xy plane (the plane of scattering); this is called a π setting. If \mathbf{d} is perpendicular to \mathbf{h} ($hk0$ reflections in K_2PtCl_4) it is moved into coincidence with the z axis by a further rotation of $\pm 90^\circ$ of ψ ; this is called a σ setting.

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Symmetry of Bicrystals Corresponding to a Given Misorientation Relationship

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Abstract

A methodology is described that enables the determination of symmetry groups of bicrystals manufactured from a given dichromatic complex. The dichromatic symmetry group is sectioned by a unique two-sided plane corresponding to the planar grain boundary and the symmetry elements of the bicrystal are established as those symmetry elements of the dichromatic group that leave the sectional plane invariant. The procedure is employed for investigating generic relations for bicrystals whose components have a given misorientation relationship. It is demonstrated that, for a dichromatic complex with point symmetry

higher than 1, bicrystals of identical symmetry can be created by more than one crystallographically equivalent interfacial plane. Finally, a new scheme is proposed for the classification of grain boundaries. This scheme provides a comprehensive framework for describing the variation of bicrystal symmetry due to changes in the orientation and/or position of the associated interfacial plane.

1. Introduction

Grain boundaries are two-dimensional features separating two misorientated and displaced crystals of identical structure. In the crystallographic framework of grain-boundary symmetry (Pond &

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Bollmann, 1979; Pond & Vlachavas, 1983) the interface is considered to be planar so that we have three-dimensional configurations consisting of two semi-infinite crystals joined together at the planar interface. The starting point in the treatment of grain-boundary symmetry is the concept of the dichromatic complex that is defined as the configuration of two infinite crystals interpenetrated so that their spatial relationship corresponds to the relationship characterizing the particular grain boundary. The desired relative orientation (misorientation) and relative translation is obtained by rotating and shifting one crystal relative to the other, which is kept fixed in space. An ideal bicrystal is then manufactured by introducing a mathematical plane into the dichromatic complex in the orientation and position of the chosen interface and rejecting the atoms of one crystal on one side of the interface and the atoms of the other crystal on the other side.

The symmetry of the bicrystal depends, in general, on the symmetry of the adjacent crystals, their relative translation and rotation, the position and orientation of the interfacial plane. The effect of all but the last two of these factors on the bicrystal symmetry has been previously studied by Pond (1977), Pond & Bollmann (1979) and Vlachavas (1984*a, b*). In the present paper we will investigate changes of the bicrystal symmetry caused by varying the orientation and position of the interface. In the following a methodology is described enabling us to determine the symmetry of any bicrystal manufactured from a given dichromatic complex. Thus, we can employ the spatial arrangement implied by the dichromatic complex for recognizing at once all the interfacial planes associated with different bicrystal symmetries. Also, the presented approach allows us to establish the relationships between interfacial planes giving the same bicrystal symmetry.

The symmetry of dichromatic complexes and bicrystals is described, as suggested by Pond & Bollmann (1979), by means of two-coloured symmetry groups. For this, one of the crystals of the dichromatic complex is designated black and the other white; the latter is taken as the reference crystal. Symmetry operations that leave the white and black crystals invariant correspond to ordinary symmetry operations and those that relate white to black, or *vice versa*, are associated with antisymmetry (or colour-reversing symmetry) operations.

2. The principle of the method

The formation of an ideal bicrystal causes the symmetry of the corresponding dichromatic complex to be lowered and this is represented by considering that the dichromatic complex is sectioned by a unique plane, called sectional plane. The orientation of the

sectional plane in the dichromatic complex is the same with the orientation of the interfacial plane of the desired bicrystal. Furthermore, for taking into account the reduction of symmetry implied by the presence of atoms of different colours on either side of the interface, the sectional plane is considered two-sided by assuming that one of its sides is coloured white and the other black. In this paper, the normal to the interfacial plane is taken to point towards the white half of the bicrystal.

It is clear that the symmetry of a bicrystal is allowed to contain only those of the symmetry elements (symmetry axes and symmetry planes) that are common in the symmetry groups of the dichromatic complex and the two-sided sectional plane. So, strictly speaking, the symmetry of the bicrystal is described by a subgroup of the symmetry group of the dichromatic complex. The kind and/or order of the symmetry elements of this subgroup must be consistent with the requirement of invariance of the interfacial plane and this implies that:

- (1) no ordinary centre of inversion is consistent with a bicrystal whereas the colour-reversing centre of inversion must be 'in' the interfacial plane.
- (2) perpendicular to the interfacial plane: either three-, four- and sixfold colour-reversing rotoinversion axes* or ordinary symmetry elements of order two, three, four and six.
- (3) parallel to the interfacial plane: only twofold proper or improper colour-reversing symmetry rotations.
- (4) inclined to the plane: no symmetry elements.

Bicrystals may have zero-, one- or two-dimensional periodicity depending on the number of non-collinear translation axes there are on the interfacial plane (Pond & Bollmann, 1979). The presence and disposition of the translational symmetry elements of a bicrystal are restricted by the periodicity of the dichromatic complex and the orientation of the sectional plane in the dichromatic complex. In the following sections the dichromatic complex is taken to have three-dimensional translational symmetry, that is, it corresponds to those misorientations of the two crystals for which a coincidence-site lattice (CSL) is formed. These misorientations are described by a rotation angle θ along a direction $[uvw]$, where $[uvw]$ is expressed in the unit cell of the white crystal, and they are symbolized by $[uvw]/\theta$. For bicrystals manufactured from CSL dichromatic complexes, rational sectional planes possess two-dimensional translational symmetry whereas irrational planes may correspond to one- or zero-dimensional periodic bicrystals.

* Although only examples of $\bar{1}'$ (which by themselves are rather special cases; Vlachavas, 1980) have come to the author's notice, all the rotoinversion axes are considered for the sake of generality.

3. Bicrystal point symmetry

The first step in the determination of the symmetry of bicrystals manufactured from a given dichromatic complex is to establish all the interfacial orientations of possible interest. This is carried out by introducing the sectional plane in the point group of the dichromatic complex. The origin of this group represents an invariant point on the sectional plane and, consequently, this procedure yields the highest point symmetry of bicrystals corresponding to different orientations of the interfacial plane. For this, we select first from all the subgroups* of the dichromatic point group only those that are permissible bicrystal point groups (Pond & Vlachavas, 1983). Then, for each of the selected subgroups we establish the orientation of the sectional plane so that all colour-reversing symmetry elements lie within this plane and all ordinary elements are perpendicular to the plane (except for colour-reversing rotoinversion axes; see above).

For the determination of the interfacial plane orientation, it is advisable to consider the subgroup list in the sequence of decreasing group order. The reason for this is that in some cases the same orientation of the sectional plane corresponds to two, or more, subgroups of the dichromatic point group. But for these planes the lower-order groups are subgroups of the bicrystal symmetry associated with the particular orientation of the interface.

An example will serve to demonstrate the deviation of the interfacial orientations of possible interest and the corresponding highest bicrystal point symmetries. We consider the dichromatic pattern† formed by two face-centred cubic lattices in the $[001]/36.9^\circ$ CSL misorientation (Fig. 1); the space group of this pattern is $I4/m\bar{m}'m'$. The subgroups of $4/m\bar{m}'m'$ that correspond to permissible bicrystal point groups are: $42'2'$ (1), 4 (1), $m'm'2'$ (4), $22'2'$ (2), m' (4), $2'$ (4), m (1), 2 (1), 1 (1), where the numbers in parentheses represent the total number of subgroups. The determination of interfacial planes for these subgroups is summarized in Table 1. Its first column lists the permissible bicrystal point groups. The second and third columns give the number and orientation of the crystallographically equivalent groups corresponding to each subgroup of $4/m\bar{m}'m'$ appearing in the first column. The last column tabulates the orientation of the interfacial plane of each bicrystal group. The

* This includes the crystallographically equivalent as well as the trivial subgroups. By way of introduction we have chosen to treat each crystallographically equivalent subgroup separately, although, as will be shown in § 6, the interfacial planes associated with a set of symmetry-equivalent subgroups can be determined by means of simple group-theoretical considerations.

† A dichromatic pattern is defined as the dichromatic complex formed by two interpenetrating point lattices (Pond & Vlachavas, 1983).

Table 1. *Determination of the bicrystal groups and the associated interfacial planes for the group $G = 4/m\bar{m}'m'$*

(The coordinate system for specifying the orientation of symmetry elements and interfacial planes is as indicated in Fig. 1.)

Bicrystal group H ($H \subset G$)	Number	Symmetry-equivalent subgroups H in G Orientation	Interfacial plane
$42'2'$	1	$4\ [001]_c, 2\ [100]_c$	$(001)_c$
4	1	$4\ [001]_c$	$(001)_c$
$mm'2'$	2	$m'\ (100)_c, m\ (001)_c$ $m'\ (010)_c, m\ (001)_c$	$(100)_c$ $(010)_c$
$mm'2'$	2	$m'\ (110)_c, m\ (001)_c$ $m\ (\bar{1}10)_c, m\ (001)_c$	$(110)_c$ $(\bar{1}10)_c$
$22'2'$	1	$2'\ [100]_c, 2'\ [010]_c$	$(001)_c$
$22'2'$	1	$2'\ [110]_c, 2'\ [\bar{1}10]_c$	$(001)_c$
m'	2	$m'\ (100)_c$ $m'\ (010)_c$	$(100)_c$ $(010)_c$
m'	2	$m'\ (110)_c$ $m'\ (\bar{1}10)_c$	$(110)_c$ $(\bar{1}10)_c$
$2'$	2	$2'\ [100]_c$ $2'\ [010]_c$	$(0kl)_c$ $(h0l)_c$
$2'$	2	$2'\ [110]_c$ $2'\ [\bar{1}10]_c$	$(\bar{h}hl)_c$ $(hhl)_c$
m	1	$m\ (001)_c$	$(hk0)_c$
2	1	$2\ [001]_c$	$(001)_c$
1	1	Any	$(hkl)_c$

directions and planes in Table 1 are expressed relative to the coordinate system of Fig. 1; this is indicated by the subscript c .

4. Spatial symmetry of bicrystals

The determination of the spatial bicrystal symmetry is carried out by introducing the sectional plane in the space group* of the corresponding dichromatic complex. In this case, the bicrystal symmetry depends

* Here on, we use the term 'space (symmetry) group' to indicate three-dimensional periodicity and the term 'spatial (symmetry) group' for two- or one-dimensional periodicity.

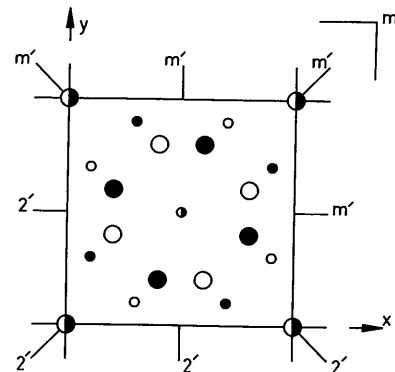


Fig. 1. Projection along $[001]$ of the unit cell of the CSL dichromatic pattern formed by two face-centred cubic lattices with misorientation $[001]/36.9^\circ$. Large and small circles represent sites at levels 0 (or 1) and $\frac{1}{2}$ along $[001]$, respectively. Open and filled circles correspond to sites of the white and black lattice, respectively. The x and y axes of the CSL coordinate system are also shown; the z axis is out of the plane of the paper.

Table 2. Two-dimensional periodic symmetry groups corresponding to sectioning of the space group $I4/mm'm'$

Orientation of sectional plane*	Elevation of sectional plane†			Periodicity of sectional plane
	$0, \frac{1}{2}$	$\frac{1}{4}, \frac{3}{4}$	Others	
$\{001\}_c$	$p42'2'$	$p42'2'$	$p411$	a, b
$\{100\}_c$	$p2'mm'$	$p2'mn'$	$p1m1$	a, c
$\{110\}_c$	$c2'mm'$	$c2'mc'$	$p1m1$	a + b, c
$\{hk0\}_c$	$p1m1$	$p1m1$	$p1m1$	
$\{h0l\}_c$	$p12'1$	$p1$	$p1$	
$\{hhl\}_c$	$p12'1$	$p1$	$p1$	
$\{hkl\}_c$	$p1$	$p1$	$p1$	

* Expressed relative to the coordinate system indicated in Fig. 1.

† Elevation is given in terms of fractional distance between the planes with listed indices (origin at $mm'm'$ intersection).

on both the orientation and the location of the sectional plane in the space group of the dichromatic complex. Parallel relocation of the interfacial plane can change the symmetry of bicrystals whose spatial group possesses colour-reversing symmetry elements since such elements are present in a bicrystal only when the particular interface location contains them. For bicrystals where the basis is a single atom, parallel relocation of the interfacial plane is not distinct from rigid-body translation, *i.e.* displacement of the black crystal relative to the white one in a direction parallel to the interfacial plane (Pond, 1977). However, if the basis is more complex this is not generally true (Pond & Vlachavas, 1983). Exceptions are, for example, interfaces in materials where the basis consists of two atoms and the basis vector (*i.e.* the vector joining the atoms in different surroundings) is parallel to the interface in question.

The procedure for determining the possible spatial groups of bicrystals is demonstrated by considering the CSL dichromatic pattern of Fig. 1. The interfacial orientations of possible interest were determined in the previous section and they are $\{100\}_c$, $\{001\}_c$, $\{110\}_c$ and so on. However, for a given orientation of the sectional plane only certain locations of this plane in the dichromatic pattern give distinct bicrystal groups. Thus, at the edge of the unit cell* of the dichromatic pattern the sectional plane $(001)_c$ corresponds to a two-dimensional periodic bicrystal with symmetry $p42'2'$. At $z = c/2$, where c is the magnitude of the periodicity vector along $[001]_c$, the plane $(001)_c$ has the same symmetry as just described. On the other hand, at $z = c/4$ or $z = 3c/4$ the sectional plane has symmetry $p42'2'$. All other locations of the sectional plane $(001)_c$ correspond to bicrystals with symmetry $p4$. It must be recalled that the ordinary symmetry operations of a bicrystal, being always perpendicular to the interfacial plane, are invariant with parallel relocation of the interface.

* The origin of the unit cell is taken at the $mm'm'$ intersection of the group $I4/mm'm'$.

The bicrystal symmetry groups obtained by sectioning the space group $I4/mm'm'$ in various orientations and positions are listed in Table 2. The symbols of the planar symmetry groups in this table are given according to the international coordinate system (see *e.g.* Pond & Vlachavas, 1983). In the last column of Table 2 the two-dimensional periodicity of the bicrystal groups enclosed in the top two frames is expressed in terms of the vectors **a**, **b**, **c** ($|\mathbf{a}| = |\mathbf{b}|$) of the unit cell of the dichromatic pattern. The reason for considering these groups only will become apparent in the next section.

5. A new scheme for the classification of interfaces

Changes of the orientation and/or the position of the interfacial plane modify both the point and the translational symmetry of a bicrystal. The periodicity and the ordinary symmetry elements of a bicrystal are invariant with respect to parallel relocation of the interface. Thus, variations in the position of the interfacial plane, affecting the colour-reversing symmetry elements only, can alter the point group of a bicrystal while conserving its translational symmetry. On the other hand, changes in the orientation of the interfacial plane affect both the (ordinary and colour-reversing) symmetry operations and the periodicity of a bicrystal.

Accordingly, interfaces can be classified into four categories. The first category comprises the interfaces for which the bicrystal symmetry group is uniquely determined by the orientation and position of the sectional plane. Examples of such interfaces are shown in the top left frame of Table 2. These will be called 'completely rigid interfaces' since when the sectional plane is rotated by an arbitrarily small angle about any direction and/or displaced by an arbitrarily small distance along its normal the corresponding bicrystal symmetry changes. The second category contains interfaces corresponding to bicrystals whose symmetry remains invariant with respect to arbitrary changes of the orientation and/or position of the interface. Such interfaces are called 'non-rigid interfaces' and they are not enclosed in any frame in Table 2.

In the third category we have interfaces for which the bicrystal symmetry implies that only the interfacial orientation is uniquely determined. Sectional planes parallel to a well defined orientation of the dichromatic complex, say $(001)_c$, $(110)_c$ *etc.*, are characteristic of this category. Examples are shown in the top right frame of Table 2 and they are called 'orientation-rigid interfaces'. Finally, interfaces for which the corresponding bicrystal symmetry is invariant with respect to the orientation but not to parallel relocation of the interfacial plane are called 'elevation-rigid interfaces' and are shown in the bottom left frame in Table 2.

In general, if the bicrystal symmetry group implies the specification of two (three) crystallographic directions of the dichromatic complex, then the interface will be either completely rigid or orientation-rigid. In this case, the periodicity of the associated bicrystals is uniquely defined by the orientation of the sectional plane. On the other hand, if the bicrystal group necessitates the definition of a single direction or is not connected with any direction (as for 1 and $\bar{1}'$) then the interface will be elevation-rigid or non-rigid. For these interfaces, the number of non-collinear periodicity axes of the corresponding bicrystal depends on the orientation of the sectional plane. If this plane is parallel to a rational plane of the dichromatic complex, then the bicrystals obtained exhibit two-dimensional periodicity. If, however, the boundary plane is irrational, the bicrystals possess either one-dimensional translational symmetry or they are aperiodic.

6. Symmetry-related interfaces

As was mentioned in § 2, the formation of a bicrystal is accomplished by a reduction in symmetry and, as a consequence, sets of bicrystals of identical symmetry can be created by more than one crystallographically equivalent interfacial plane.* The bicrystals of such sets are called 'symmetry-related bicrystals' and they occur whenever a dichromatic complex contains point symmetry higher than 1 and the order of the bicrystal point group is less than the order of the dichromatic point group.

It can be easily shown, following somewhat similar considerations to that of Aizu (1970) and Tendeloo & Amelinckx (1974), that the mutual relationships between symmetry-related bicrystals are described by decomposing the dichromatic point group G into (left) cosets of the bicrystal point group H ($H \subset G$):

$$G = g_1H + g_2H + \dots + g_nH,$$

where the g_i are not elements of H (except of the identity operation g_1). Then, each coset represents the complete set of operations leading from a given bicrystal to another symmetry-related bicrystal. This implies that:

- (1) the number of symmetry-related bicrystals of given symmetry is equal to the index of H in G ;
- (2) the set of operations that generates all symmetry-related bicrystals can be obtained by taking one operation from each coset in the development of G into cosets of H .

For the example considered in §§ 4 and 5 we have $G = 4/mm'm'$; and let $H = 42'2'$. Since H is a subgroup of index 2 of G , we have $G = H + iH$, where i is the

ordinary inversion operation, and this means that in this case two symmetry-related bicrystals exist. Each bicrystal has symmetry H and in both bicrystals the elements of H have the same orientation because H is an invariant subgroup of G . The relationship between the two bicrystals is described by any symmetry operation of the coset iH . The same symmetry operations relate the interfacial planes of the two bicrystals, which are the $(001)_c$ and $(00\bar{1})_c$ planes, respectively, passing through the origin of the unit cell of the dichromatic pattern. It must be recalled that the specification of the interfacial plane determines the orientation as well as the white and black sites of the plane.

Consider now that $H = mm'2'$ with $m \parallel (001)_c$, $m' \parallel (100)_c$. The symmetry relations of the bicrystals corresponding to this orientation of H are determined by the decomposition $G = H + C_1 + C_2 + C_3 = \{1, s'_{100}, s_{001}, 2'_{010}\} + \{s'_{110}, 4'_{001}, 2'_{110}, 4'_{001}\} + \{s'_{110}, 4'_{001}, 2'_{110}, 4'_{001}\} + \{2'_{001}, s'_{010}, i, 2'_{100}\}$ (the symmetry-operation notation has been explained by Vlachavas, 1984b). We have four symmetry-related bicrystals V_1, V_2, V_3, V_4 (Fig. 2). Any one operation in C_1, C_2, C_3 transforms V_1 to V_2, V_3, V_4 , respectively. Therefore, the bicrystals are related by the operations of the group, say, $m'm'2 = \{1, s'_{110}, s'_{110}, 2'_{001}\}$ and the same operations relate the associated interfacial planes $(100)_c, (010)_c, (\bar{1}00)_c, (0\bar{1}0)_c$.

7. Summary

A methodology for the determination of all bicrystal symmetry groups that can be created from a given dichromatic complex has been described. The procedure is based on the restrictions imposed on the orientation of the ordinary and colour-reversing sym-

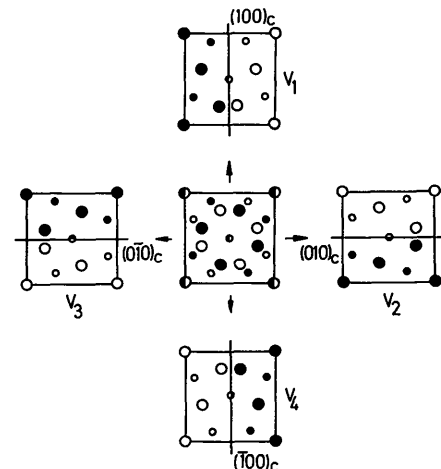


Fig. 2. [001] projection of the four variants with symmetry $p2'mm'$ obtained by locating the sectional plane parallel to $\{100\}_c$ with elevation 0 in the dichromatic pattern of Fig. 1. Large and small circles represent sites at levels 0 (or 1) and $\frac{1}{2}$ along the projection direction, respectively.

* It is possible that bicrystals with identical symmetry can be created by crystallographically non-equivalent interfacial planes. These cases, however, must be treated separately.

metry elements of a bicrystal. The former must always be perpendicular to the interfacial plane and the later parallel to it (except of colour-reversing rotoinversion axes; see § 2). In order to take into account these restrictions, we consider that the symmetry group of the dichromatic complex is sectioned by a unique two-sided plane. Thus, the symmetry of the bicrystal associated with the particular orientation of the interfacial plane is expressed by the set of symmetry operations of the dichromatic group that leave the two-sided sectional plane invariant. This procedure provides us with a comprehensive method for investigating generic relations amongst bicrystals corresponding to the same misorientation relationship of their components.

The most important conclusion achieved by studying the bicrystal symmetry by this method is that crystallographically equivalent interfacial planes create bicrystals with symmetry-related structures. Symmetry-related bicrystals arise as a consequence of dissymmetrization, and in this respect the idea of regarding a bicrystal as having been created by sectioning the corresponding dichromatic complex is most helpful.

Further examination of generic relations amongst bicrystals can be accomplished by employing the

proposed classification of interfaces. The distinction of four types of interfaces, namely completely rigid, orientation-rigid, elevation-rigid and non-rigid interfaces, is important in connection with the physical properties of bicrystals. For the first three types of interfaces a small deviation from the orientation and/or position of the corresponding interfacial plane may be related to a sharp transition in the properties of the bicrystals. On the other hand, the symmetry considerations presented in this paper indicate that non-rigid interfaces can exhibit smooth changes of their physical properties over a wide range of interfacial orientations.

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Pseudo-Weak-Phase-Object Approximation in High-Resolution Electron Microscopy.

I. Theory

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Abstract

On the basis of the dynamical electron diffraction theory of Cowley & Moodie [*Acta Cryst.* (1957), **10**, 609–619], a new formula has been derived for the multiple-beam image intensity expressed in terms of the projected potential distribution as well as the specimen thickness. According to this formula, crystals for which the weak-phase-object approximation does not hold can be treated by the pseudo-weak-phase-object approximation (PWPOA) up to a certain critical thickness. Here the real crystal is replaced by its imaginary isomorph, where the constituent heavy atoms behave as lighter atoms than those of the real crystal, and *vice versa*. The validity of the PWPOA is discussed and confirmed by the comparison of the images of chlorinated Cu phthalocyanine calculated with PWPOA and the multislice method.

1. Introduction

According to the weak-phase-object approximation (WPOA) the image intensity is expressed as

$$I(x, y) = 1 - 2\sigma\varphi(x, y) \quad (1.1)$$

under the optimum defocus condition (Scherzer, 1949; Cowley & Iijima, 1977), where $\sigma = \pi/\lambda E$, λ is the wavelength of electrons, E the accelerating voltage and $\varphi(x, y)$ the projection of the potential distribution function (PPDF) of the weak phase object along the beam direction. Formula (1.1) shows a linear relationship between the image intensity and the PPDF. But it is well known that structure images corresponding to the projection of the crystal structure can be obtained with specimens considerably thicker than the WPOA holds for. This was inter-