The matrices $R$ have the following matrix form:

$$
R^1 = \begin{bmatrix} 2 & 0 & 0 \\ 1 & 0 & 2 \\ 1 & 2 & 0 \end{bmatrix}, \quad R^2 = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix},
$$

$$
R^3 = \begin{bmatrix} 2 & 0 & 0 \\ 1 & 1 & 2 \\ 0 & 1 & 0 \end{bmatrix}, \quad R^4 = E.
$$

$R^2$ is the $C_{2h}$ element and we may construct $G_{A_1}$ by making use of the $C_{2h}$ element. Therefore,

$$
G_{A_1} = \{ R, R^2, R^3, R^4 \} + C_2 \{ R, R^2, R^3, R^4 \}
$$

$$
= \{ E, C_{2h}, C_{2h}, C_2, R, R^{-1}, C_2 R, C_2 R^3 \}
$$

and $G_{A_1}$ is isomorphic to the $D_4$ tetragonal symmetry group.

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**References**


nately, there are computational difficulties and ambiguities in this procedure, which have been mentioned by other authors, who proposed different algorithms of a more general character (Bonnet & Durand, 1975; Bonnet, 1976; Karakostas, Nouet & Delavignette, 1979).

In this paper we present a method for the calculation of the DSCL base using the symmetry properties of the CSL (Doni, Bleris, Karakostas, Antonopoulos & Delavignette, 1985).† A general procedure is presented, which reduces the DSCL computation to the determination of some analytical expressions, allowing the construction of a primitive DSCL base for every CSL of the given crystal system in a very simple way. Moreover, both CSL and DSCL are referred to the same coordinate system, which is a considerable help for the experimental study of GBs.

2. The basic idea

According to Grimmer’s theorem, the DSCL can be defined if a base \([x^*]\) of the reciprocal coincidence lattice of a given CSL is known (Grimmer, 1974). In fact, the DSCL base \([x]\) is connected with the \([x^*]\) base by the relation

\[ [x] = ([x^*])^{-1} [x^*], \]

which expresses the reciprocity theorem.

From (1) it is obvious that the problem of determining the DSCL is simply equivalent to the calculation of the base \([x^*]\). Noting by CSL the direct coincidence lattice and by CSL* its reciprocal, we shall use the same notation as in paper I for the different quantities, using a star when they are referred to the CSL*.

Thus, for the determination of \([x^*]\) it is enough to know the rotation matrix \(R^*\) and a base \([x^*]\)_1 of CSL*.

From (1) it is obvious that we can have a primitive CSL* base if we can find among the different \(r^*_j\) vectors three vectors with volume equal to \(\Sigma\), i.e. the multiplicity of the CSL, which remains the same for the CSL*.

If we take into account that the CSL properties, which are used in the theoretical treatment given by Bleris (1983), are still valid for the CSL*, we can say that there is always a solution between the different eigenvectors of the symmetrically equivalent rotation matrices.

What remains to be found are the analytical expressions of the different eigenvectors. We shall examine the cubic and the hexagonal systems, since for those two systems all the information concerning the symmetry has already been published in paper I. A comparison of our results can be made with the data given by Grimmer et al. (1974) for the cubic and by Bonnet, Cousineau & Warrington (1981) for the hexagonal systems.

3. Cubic system

For the simple cubic lattice direct and reciprocal-space vectors are expressed by the same indices and the rotation matrix \(R^* = R\). The analytical form of this matrix has been extensively studied by Bleris & Delavignette (1981). They have shown that the elements of the matrix are a function of the multiplicity of the CSL, \(\Sigma\), of the Miller indices of the rotation axis, \(u, v, w\), and of three integer parameters \(m, n, \alpha\) whose conditions limiting their possible values have been established. The matrix elements, as a function of

\[ \Sigma, u, v, w, m, n, \alpha \]

allow an easy determination of all possible CSLs. Its expression is given in equation (31a) of Bleris & Delavignette (1981). By computing the products

\[ R_j = g_j R, \quad j = 1, 2, \ldots, 24, \]

where \(g_j\) is the \(3 \times 3\) matrix representation of the symmetry elements of the cubic system given by Karakostas, Bleris & Antonopoulos (1979), we can take the analytical expressions of the symmetrically equivalent descriptions of the given CSL. In Table 1 the relation

\[ \alpha \Sigma \cos^2 \theta/2 \]

as well as the indices of the rotation axis for each of the equivalent descriptions as functions of the integer numbers of (7) are tabulated. The rotation angle \(\theta\) can easily be obtained from (9).

The information given by this table can be used beyond our main purpose. For example, this classifi-
Table 1. Angles and rotation-axis indices of the different descriptions of the cubic CSLs

<table>
<thead>
<tr>
<th></th>
<th>aΣ cos² (θ/2)</th>
<th>α</th>
<th>υ</th>
<th>δ</th>
<th>ζ</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>m²</td>
<td>u</td>
<td>w</td>
<td>v</td>
<td>w</td>
</tr>
<tr>
<td>2</td>
<td>(un - m)²/2</td>
<td>v</td>
<td>(u - v)w</td>
<td>(u - v)w</td>
<td>(u - v)w</td>
</tr>
<tr>
<td>3</td>
<td>(un - m)²/2</td>
<td>u</td>
<td>(u - v)w</td>
<td>(u - v)w</td>
<td>(u - v)w</td>
</tr>
<tr>
<td>4</td>
<td>(w n - m)²/2</td>
<td>w</td>
<td>-w</td>
<td>-w</td>
<td>-w</td>
</tr>
<tr>
<td>5</td>
<td>(un + m)²/2</td>
<td>u</td>
<td>(u - v)w</td>
<td>(u - v)w</td>
<td>(u - v)w</td>
</tr>
<tr>
<td>6</td>
<td>(vn + m)²/2</td>
<td>u</td>
<td>(u - v)w</td>
<td>(u - v)w</td>
<td>(u - v)w</td>
</tr>
<tr>
<td>7</td>
<td>(wn + m)²/2</td>
<td>u</td>
<td>(u - v)w</td>
<td>(u - v)w</td>
<td>(u - v)w</td>
</tr>
<tr>
<td>8</td>
<td>((u + v + w)² - m)²/2</td>
<td>v</td>
<td>(u - v)w</td>
<td>(u - v)w</td>
<td>(u - v)w</td>
</tr>
<tr>
<td>9</td>
<td>((u + v - w)² + m)²/2</td>
<td>u</td>
<td>(u - v)w</td>
<td>(u - v)w</td>
<td>(u - v)w</td>
</tr>
<tr>
<td>10</td>
<td>((u - w)² + m)²/2</td>
<td>w</td>
<td>-w</td>
<td>-w</td>
<td>-w</td>
</tr>
<tr>
<td>11</td>
<td>((u - v)² + m)²/2</td>
<td>u</td>
<td>(u - v)w</td>
<td>(u - v)w</td>
<td>(u - v)w</td>
</tr>
<tr>
<td>12</td>
<td>((u - v)² + m)²/2</td>
<td>u</td>
<td>(u - v)w</td>
<td>(u - v)w</td>
<td>(u - v)w</td>
</tr>
<tr>
<td>13</td>
<td>((v - w)² + m)²/2</td>
<td>v</td>
<td>(u - v)w</td>
<td>(u - v)w</td>
<td>(u - v)w</td>
</tr>
<tr>
<td>14</td>
<td>((w - v)² + m)²/2</td>
<td>w</td>
<td>-w</td>
<td>-w</td>
<td>-w</td>
</tr>
</tbody>
</table>

Table 2. The smallest values of the determinants of the vectors of Table 1 in triplets

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>(u - v)αΣ</td>
<td>(u - v)αΣ</td>
<td>(u - v)αΣ</td>
<td>(u - v)αΣ</td>
</tr>
<tr>
<td>(u - w)αΣ</td>
<td>(u - w)αΣ</td>
<td>(u - w)αΣ</td>
<td>(u - w)αΣ</td>
</tr>
<tr>
<td>(v - w)αΣ</td>
<td>(v - w)αΣ</td>
<td>(v - w)αΣ</td>
<td>(v - w)αΣ</td>
</tr>
</tbody>
</table>

The computational algorithm for the construction of the DSCL base is now reduced to the following procedure:

(i) We compute all the axis-angle pairs of the symmetrically equivalent descriptions by using Table 1.

(ii) From the 24 axes we take all the combinations of three vectors by keeping the first axis invariant.

(iii) From their determinants we choose a triplet with volume equal to Σ. This triplet defines a primitive base of Α.1.

(iv) We apply to this triplet the matrix R of the smallest angle (or the first) description and a primitive DSCL base can be obtained by taking the inverse transpose of the result.

With these four steps, which take a few seconds on a personal computer, a primitive base can always be defined. Moreover, it should be pointed out that in step (iii) we can take all the triplets of volume equal to Σ and choose from them the one with the shortest vectors, as well as take into account the symmetry of the CSL that can give us a conventional base.

We will now consider an example, following a step by step procedure, where the symmetry has been taken into account. The Σ = 13a CSL with smallest-angle description data

\[ u = 1; v = 0; w = 0; m = 5; n = 1; α = 2 \]

(10) gives the results of Table 3 by using the relations of Table 1.

From Table 3 we can choose a triplet, taking into account that the Σ = 13a CSL has tetragonal sym-
4. Hexagonal system

The previous analysis for the cubic system is more or less of academic interest, since the cubic CSLs have been investigated by many authors. The hexagonal CSL and DSCL, however, are still under investigation, as can be seen from the recent literature (Fortes, 1983; Grimmer & Warrington, 1983). Thus, the application of the previous theoretical treatment to the hexagonal system is of great interest.

The only difficulty for the hexagonal system is the difference between direct and reciprocal space. This means that we have to find first the symmetry-equivalent rotation matrices for the direct space and then the reciprocal ones, by using (3).

The general expression of the rotation matrix has been established by Bleris, Nouet, Hagège & Delavignette (1982). The elements are functions of the parameters \( \mu \) and \( \nu \), where \( \mu / \nu = (c/a)^2 \), and the same parameters as presented for the cubic case. The rotation matrix has been given in equation (25) of Bleris et al. (1982). Also, the expression for the smallest-rotation-angle description has been given. The symmetry elements have been given by Hagège, Nouet & Delavignette (1980). From those, we have determined all the matrices

\[
R_j = g_j R, \quad j = 1, 2, \ldots, 12. \tag{14}
\]

Their eigenvectors and the corresponding \( \cos^2 \theta/2 \) expressions are given in Table 4. This classification is also presented for the first time and some useful results can be directly obtained. We know that for \( m = 0 \) the rotation angle is equal to 180° (Bleris et al., 1982). By putting \( m = 0 \) in Table 4, we take three cases where the corresponding axis has one index equal to zero, i.e., cases 10, 11, 12 (Table 4). Reciprocally, if we choose a description around an axis with an index equal to zero, then there is at least one description of 180°, as can be easily deduced from expressions 10, 11, 12 for the angles. We can also see that if it happens to be \( 2u = v \), there will be a 180° description (case 6). Moreover, many other cases could be obtained by a combination of the previous ones or by a systematic investigation of the different cases arising from the different values the integer numbers \( u, v, m, n, \alpha, \mu, \nu \) may have.

For the reciprocal-space CSL the rotation matrix \( R^* \) of the smallest-angle description has the usual form:

\[
R^* = (1/\Sigma)[r^*/\alpha]; \tag{15}
\]
Table 5. Rotation-axis indices of the different descriptions of the hexagonal CSLs in the reciprocal space

<table>
<thead>
<tr>
<th>$u^*$</th>
<th>$v^*$</th>
<th>$w^*$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$(2u-v)v$</td>
<td>$2w\mu$</td>
</tr>
<tr>
<td>2</td>
<td>$(u-v)\nu v\nu$</td>
<td>$(m+\nu)\mu$</td>
</tr>
<tr>
<td>3</td>
<td>$(u-2v)\nu (u+v)\nu$</td>
<td>$(3m+\nu)\mu$</td>
</tr>
<tr>
<td>4</td>
<td>$-vn\nu v\nu$</td>
<td>$2m\mu$</td>
</tr>
<tr>
<td>5</td>
<td>$-(u+v)\nu (2u-v)\nu$</td>
<td>$(3m+\nu)\mu$</td>
</tr>
<tr>
<td>6</td>
<td>$-vn\nu (u-v)\nu$</td>
<td>$(m+\nu)\mu$</td>
</tr>
<tr>
<td>7</td>
<td>$-2wn\nu wn-3m\nu$</td>
<td>$(2u-v)\nu n$</td>
</tr>
<tr>
<td>8</td>
<td>$-(3m+\nu)\nu wn$</td>
<td>$2wn\nu n$</td>
</tr>
<tr>
<td>9</td>
<td>$3m-wn\nu (u-v)\nu n$</td>
<td>$(u+v)n$</td>
</tr>
<tr>
<td>10</td>
<td>$2m-3m\nu wn\nu n$</td>
<td>$(2v-w)\nu n$</td>
</tr>
<tr>
<td>11</td>
<td>$m-wn-2m\nu wn\nu n$</td>
<td>$(m-\nu)\mu n$</td>
</tr>
<tr>
<td>12</td>
<td>$-(wn+m)\nu wn-m\nu n$</td>
<td>$(u-v)\nu n$</td>
</tr>
</tbody>
</table>

and the integer expressions $r^*_j$ have the following forms:

$$r^*_{1} = (2u-v)uv^2 - 2w\mu mn + 3\mu m^2 - dn^2$$
$$r^*_{2} = (2u-v)uv^2 - 4w\mu mn$$
$$r^*_{3} = [(2u-v)vn^2 + 3\nu mn]v$$
$$r^*_1 = (2u-u)uv^2 + 4w\mu mn$$
$$r^*_2 = (2v-u)uv^2 + 2w\mu mn + 3\mu m^2 - dn^2$$
$$r^*_3 = [(2u-v)wn^2 - 3\nu mn]v$$
$$r^*_{1} = [2uvn^2 + 2(u-2v)mn]\nu$$
$$r^*_{2} = [2vwn^2 + 2(2u-v)mn]\mu$$
$$r^*_{3} = 2w^2\mu^2 + 3\mu m^2 - dn^2$$

and

$$d = (u^2 + v^2 - uv)\nu + \mu w^2,$$

where $u$, $v$, $w$, $m$, $n$, $\alpha$, $\mu$, $\nu$ are the integer numbers describing the given CSL in the direct space. The different rotation axes $r^*_j, j = 1, 2, \ldots, 12$, of the CSL* symmetrically equivalent descriptions are given in Table 5. The smallest values of the determinants of their combinations in triplets are given in Table 6. We should like to point out that since the values of the parameter $\alpha$ are variable depending on the $\mu$, $\nu$ values, the $\alpha$ value can always be eliminated from the expressions of the rotation-axis indices. Thus, from the values of Table 6 and using the previous classification [see divisibility rules in Bleris et al. (1982)], we can have the following cases of divisibility.

A. $(3\mu m^2, dn^2) \div 1$

(i) If $\alpha = 2$ and $\nu \equiv 0 \text{mod} 2$, the vectors $r^*_1, r^*_4$ have even indices.

(ii) If $\alpha = 4$ and $\nu \not\equiv 0 \text{mod} 2$, then

$u = 0 \text{mod} 2$, $v = 0 \text{mod} 2$, $w = 1 \text{mod} 2$

$m = 1 \text{mod} 2$, $n = 1 \text{mod} 2$

and the indices of all the $r^*_j$ vectors are even numbers.

Table 6. The smallest values of the determinants of the vectors of Table 5 in triplets

<table>
<thead>
<tr>
<th>$\nu(2u-v)\alpha\Sigma$</th>
<th>$\nu(u-v)\alpha\Sigma$</th>
<th>$\nu\alpha\Sigma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\nu(2u-v)\alpha\Sigma$</td>
<td>$\nu(u-v)\alpha\Sigma$</td>
<td>$\nu\alpha\Sigma$</td>
</tr>
</tbody>
</table>

B. $(3\mu m^2, dn^2) \div p(p \neq 1)$

(i) If $(3, d) \div 3$, then

$u + v = 0 \text{mod} 3$, $w = 0 \text{mod} 3$, $(u, v) \not\equiv 1$

and

$2u - v = 0 \text{mod} 3$, $2v - u = 0 \text{mod} 3$.

In this case the vectors $r^*_1, r^*_3, r^*_5, r^*_6, r^*_8$ have indices that are multiples of 3.

(ii) If $(\mu, n) \equiv q(q \neq 1)$, then there are two possibilities: either

$\alpha = 0 \text{mod} 3$, with $\mu = 0 \text{mod} 3$ and $(u, v) \equiv 1$

or

$\alpha = 0 \text{mod} q$, with $(u, v) \equiv 1$.

The first case is similar to B(i) and the second one implies that, for $j = 1, 2, \ldots, 6$, the $r^*_j$ vectors have indices that are multiples of $q$.

(iii) If $(m, d) \equiv t(t \neq 1)$, then there are again two possibilities: firstly, $t = 2$ and $\mu = 0 \text{mod} 2$ and, secondly, $t \not= 2$ and $w = 0 \text{mod} t$. For the first case the parameter $\alpha$ can be eliminated from the first six vectors, and for the second case we have $\nu = 0 \text{mod} t$ and $\alpha$ is eliminated from the $r^*_j$ vector.

(iv) If $(3, n) \equiv 3$, $\alpha$ is eliminated from the vectors $r^*_1, r^*_3, r^*_5$.

(v) If $(\mu, n) \equiv p(p \neq 1)$, $\alpha$ can be eliminated from the first six vectors of Table 5.

From the above analysis we can ensure that there are always some combinations of three vectors forming a primitive cell. If there is not such a possibility, we can choose two triplets that correspond to a non-primitive CSL* base and define from them a non-primitive one (Bleris, 1983).

Example: In order to show the procedure for the case of non-primitive cells, we have chosen a trivial hexagonal CSL, which exists for any $(\mu, u)$ value but for which the following values are considered:

$\Sigma = 13$, $\mu = 8$, $\nu = 3$, $m = 7$, $n = 3$, $\alpha = 96$.

and

$[uvw] = [001]$.

For this CSL the triplets with the vectors $(r^*_1, r^*_3, r^*_5)$ and $(r^*_3, r^*_5, r^*_1)$ give determinants with values

$$\text{det} [(r^*_1), (r^*_3), (r^*_5)] = 4w\alpha\Sigma = 4 \times 1 \times 96 \times 13 = 4992$$

$$\text{det} [(r^*_1), (r^*_5), (r^*_3)] = -2w\alpha\Sigma = -2 \times 1 \times 96 \times 13 = -2496.$$
The coordinates of these vectors are obtained from Table 5:

\[ r^*_1: (0, 0, 16) \]
\[ r^*_2: (24, 6, 0) \]
\[ r^*_3: (14, 10, 0) \]
\[ r^*_4: (4, 14, 0). \]

By eliminating the common factors, we end up with the following bases:

\[
B^*_1 = \begin{bmatrix} 0 & 4 & 2 \\ 0 & 1 & 7 \\ 1 & 0 & 0 \end{bmatrix}, \quad B^*_2 = \begin{bmatrix} 0 & 7 & 2 \\ 0 & 5 & 7 \\ 1 & 0 & 0 \end{bmatrix},
\]

with determinants

\[
\det [B^*_1] = 2 \times 13 \quad \text{and} \quad \det [B^*_2] = -3 \times 13.
\]

By solving the equation

\[ 2x - 3y = 1 \]
we have two obvious solutions: \((x, y) = (5, 3)\) and \((x, y) = (2, 1)\). From these we may have the following cases:

\[
B^*_1' = \begin{bmatrix} 0 & 4 \times 5 + 3 \times 7 & 2 \\ 0 & 1 \times 5 + 3 \times 5 & 7 \\ 1 & 0 & 0 \end{bmatrix}, \quad B^*_1'' = \begin{bmatrix} 0 & 1 & 2 \\ 0 & 10 & 7 \\ 1 & 0 & 0 \end{bmatrix},
\]

with \(\det [B^*_1'] = 13\) and

\[
B^*_2' = \begin{bmatrix} 0 & 4 \times 2 + 1 \times 7 & 2 \\ 0 & 1 \times 2 + 1 \times 5 & 7 \\ 1 & 0 & 0 \end{bmatrix}, \quad B^*_2'' = \begin{bmatrix} 0 & 1 & 2 \\ 0 & 3 & 7 \\ 1 & 0 & 0 \end{bmatrix}.
\]

By taking the rotation matrix \(R^*\) from (15), (16) and putting in the given CSL data we can define a CSL\(^*\) base by the multiplication

\[
R^*B^*_2 = \begin{bmatrix} 8 & 7 & 0 \\ 17 & 15 & 0 \\ 0 & 13 & 0 \end{bmatrix} \frac{1}{13}, \quad \begin{bmatrix} 0 & 1 & 2 \\ 0 & 3 & 7 \\ 1 & 0 & 0 \end{bmatrix},
\]

By taking the inverse transpose of the previous matrix, which gives the product \(\Sigma \times \text{DSCL}\) with the form

\[
\begin{bmatrix} 0 & 7 & 4 \\ 0 & 5 & 1 \\ 13 & 0 & 0 \end{bmatrix},
\]

the DSCL base can be obtained.

### 5. Discussion

According to the theory that was previously established above for the cubic and hexagonal CSL, the analytical form of the CSL rotation matrix has been given as a function of the integer numbers \(u, v, w, m, n, \alpha\) and \(\mu, \nu\), which characterize a given CSL. The construction of this matrix is, in principle, possible for any crystallographic system.

Using this analytical form and the results of paper I, we present here a method for determining the DSC lattice of a given CSL using the data of the CSL itself. The advantages of this work are simply that the Euclidian algorithms used in the past for the solution of the same problem and their difficulties in the application to different crystallographic systems have been overcome. From the practical point of view, we succeeded in having analytical expressions, which can be obtained for every system if the analytical form of their rotation matrix is known. These expressions can give all the necessary information for the different descriptions of one and the same CSL.

From the previous sections of this paper, it is obvious that, using the symmetry information of paper I, we can select a unit cell in such a way that this unit cell clearly exhibits the symmetry of the CSL. This conventional choice may be a non-primitive one, \(i.e\.\) it may contain the equivalent of more than one lattice point, but it may be useful for the study of the CSL. This can be done directly by using paper I and the tables of the analytical expressions of the rotation axes of this work.

We have treated many \(\mu/\nu\) ratios of hexagonal CSLs. Comparing with relevant published results (Bonnet et al., 1981), we found very good agreement. In some cases we have the same type of vectors but different orientations. In some other cases an obvious combination gives identical results. Finally, it should be noted that the computational algorithms are very simple and very quick. Especially for the hexagonal system, where there are only 55 combinations to be taken into account, the computational time is negligible.

This work was partially supported by the Greek Ministry of Research and Technology.

### References


Phase Determination of the Forbidden Reflection 442 in Silicon and Germanium Using Multiple Bragg Scattering

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Abstract

The sign inversion of the forbidden reflection 442 in silicon between room temperature and 700 K has been verified using multiple beam diffraction and the concept of virtual Bragg scattering. A similar determination in the case of germanium confirms that the 442 is mostly due to anharmonic effects at room temperature.

It is well known that n-beam diffraction can be used, in principle, to determine phases in X-ray or neutron reflections (Colella, 1974; Post, 1977). Progress has been hindered so far by the fact that n-beam dynamical theory, the only one that preserves phase information, is strictly applicable to perfect crystals such as germanium and silicon, and it was not clear how it could be applied to real mosaic crystals. It was proposed (Chapman, Yoder & Colella, 1981), in 1981, that virtual Bragg scattering (VBS), a situation in which all interactions are deliberately kept weak, might provide a way to deal with mosaic crystals.

In practice, a VBS situation is one in which a weak reflection is fully excited and its integrated intensity is measured by varying \( \theta \), the angle of incidence on the lattice planes. At the same time one or more extra reflections are excited by choosing a suitable value for \( \varphi \), the azimuthal angle around the scattering vector, in such a way as to keep the excitation weak. In a plot of \( R_{hkl}^{\varphi} \) vs \( \varphi \), \( R_{\varphi}^{\theta} \) being the integrated intensity of the \( hkl \) reflection integrated with respect to \( \theta \) at constant \( \varphi \), a VBS situation corresponds to points on the sides of a strong Umweganregung peak, typically 2–4° away from full excitation. It has been proved in our previous work (Chapman, Yoder & Colella, 1981) that the asymmetric pattern observed around a strong Umweganregung peak contains phase information.

To test this idea in a very clear cut case, we decided to verify the phase change of the 442 reflection in silicon at two different temperatures.† The forbidden 442 reflection in silicon was measured several years ago (Trucano & Batterman, 1972), and found to...