R have the following matrix form:

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

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

R^2 is the $C'_{22}\in H_1$ element and we may construct $G_{A_1^1}$ by making use of the $C_2\in H_1$ element. Therefore,

$$G_{A_1^1}=\{R, R^2, R^3, R^4\}+C_2\{R, R^2, R^3, R^4\}$$
$$=\{E, C'_{22}, C''_{22}, C_2, R, R^{-1}, C_2R, C_2R^3\}$$

and $G_{A_1^1}$ is isomorphic to the D_4 tetragonal symmetry group.

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

References

BLERIS, G. L. & DELAVIGNETTE, P. (1981). *Acta Cryst.* **A37**, 779-786.

BLERIS, G. L., DONI, E. G., KARAKOSTAS, TH., ANTONOPOULOS, J. G. & DELAVIGNETTE, P. (1985). *Acta Cryst.* **A41**, 445-451.

BLERIS, G. L., KARAKOSTAS, TH. & DELAVIGNETTE, P. (1983). *Comput. Phys. Commun.* **28**, 287-297.

BRADLEY, C. J. & CRACKNELL, A. P. (1972). *The Mathematical Theory of Symmetry in Solids.* Oxford: Clarendon Press.

GRATIAS, D. & PORTIER, R. (1982). *J. Phys.* **43** (Suppl. to No 12), C6.15-C6.24.

GRIMMER, H., BOLLMANN, W. & WARRINGTON, D. H. (1974). *Acta Cryst.* **A30**, 197-207.

HAGÈGE, S., NOUET, G. & DELAVIGNETTE, P. (1980). *Phys. Status Solidi A*, **62**, 97-107.

International Tables for X-ray Crystallography (1969). Vol. I. Birmingham: Kynoch Press.

KARAKOSTAS, TH., BLERIS, G. L. & ANTONOPOULOS, J. G. (1979). *Phys. Status. Solidi A*, **55**, 801-809.

POND, R. C. & BOLLMANN, W. (1979). *Philos. Trans. R. Soc. London Ser. A*, **292**, 449-472.

VAN TENDELOO, G. & AMELINCKX, S. (1974). *Acta Cryst.* **A30**, 431-440.

Acta Cryst. (1985). **A41**, 445-451

Use of the CSL Symmetrically Equivalent Descriptions Tables in the DSC Lattice Base Computation

BY G. L. BLERIS, E. G. DONI AND TH. KARAKOSTAS

Physics Department, University of Thessaloniki, Thessaloniki, Greece

J. G. ANTONOPOULOS

Department of Electrical Engineering, Democritus University of Thrace, Xanthi, Greece

AND P. DELAVIGNETTE

Materials Science Department, CEN/SCK, B-2400 Mol, Belgium

(*Received* 4 *June* 1984; *accepted* 2 *April* 1985)

Abstract

A combination of analytical expressions and a knowledge of symmetry is employed for the displacement shift complete lattice (DSCL) base computation. The method is of general use and its application to cubic and hexagonal systems is given. Tables containing all the symmetrically equivalent descriptions of one and the same coincidence site lattice (CSL) as a function of one description are given for both cubic and hexagonal systems.

1. Introduction

Since the grain boundary (GB) cannot be described only on the basis of absolutely exact coincidence site lattice (CSL) orientations, the study of equilibrium grain boundaries in the vicinity of a CSL condition is a real necessity and a completion to a full CSL study. It has been experimentally shown that the deviation of a few degrees from the exact CSL condition is usually accommodated by a dislocation array. The Burgers vectors of such a dislocation array are related with the approximate CSL if they are members of the corresponding displacement shift complete lattice (DSCL) (Bollmann, 1970).

According to the reciprocity theorem, which has been established by H. Grimmer, there is a one-to-one correspondence between the CSL and the DSCL, and the DSCL base can be found if the CSL base is known (Grimmer, 1974). An application of this elegant statement, which is of general character, was given for the DSCL of the cubic system for CSLs up to $\Sigma=49$ by Grimmer, Bollmann & Warrington (1974). Unfortu-

0108-7673/85/050445-07$01.50

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 referrred 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

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

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 referrred to the CSL*. Thus, for the determination of $[x^*]$ it is enough to know the rotation matrix R^* and a base $[x^*]_1^1$ of Λ_1^{1*}, since

$$R^*[x^*]_1^1 = [x^*]_1^2 = [x^*]. \tag{2}$$

The CSL* rotation matrix R^* is easily obtained by a similarity transformation of the rotation matrix R of the corresponding CSL,

$$R^* = SRS^{-1}, \tag{3}$$

where S is the matrix transforming a vector of the direct space to one of the reciprocal space. The difficult question to be answered is how to determine the base $[x^*]_1^1$.

Let us consider the symmetrically equivalent descriptions of the CSL*, *i.e.*

$$R_j^* = g_j^* R^*, \qquad j = 1, 2, \ldots, [G^*], \tag{4}$$

where $[G^*]$ is the order of the symmetry group of the Λ_1^* lattice. We know that all the eigenvectors $\mathbf{r}_j^*$ of R_j^* are vectors of the Λ_1^{1*} sublattice. Since

$$R^*\Lambda_1^{1*} = \Lambda_1^{2*} = \Lambda_{12}^*, \tag{5}$$

we have

$$\forall\, \mathbf{r}_j^*\colon \bar{r}_j^* = R_j^*\mathbf{r}_j^* \rightarrow R^*\mathbf{r}_j^* \in \mathrm{CSL}^*. \tag{6}$$

From this last relation it is obvious that we can have a primitive CSL* base if we can find among the different $\mathbf{r}_j^*$ vectors three vectors with volume equal to Σ, *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 $R^* \equiv R$. 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, Σ, of the Miller indices of the rotation axis, u, v, w, and of three integer parameters m, n, α whose conditions limiting their possible values have been established. The matrix elements, as a function of

$$\Sigma, u, v, w, m, n, \alpha \tag{7}$$

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

$$R_j = g_j R, \qquad j = 1, 2, \ldots, 24, \tag{8}$$

where g_j is the 3×3 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

$$\alpha\Sigma \cos^2 \theta/2 \tag{9}$$

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 θ can easily be obtained from (9).

The information given by this table can be used beyond our main purpose. For example, this classifi-

† In the following, this work will be referrred to as paper I.

Table 1. *Angles and rotation-axis indices of the different descriptions of the cubic CSLs*

	$\alpha\Sigma\cos^2(\theta/2)$	u_r	v_r	w_r
1	m^2	u	v	w
2	$(un-m)^2/2$	$un+m$	$(v-w)n$	$(v+w)n$
3	$(vn-m)^2/2$	$-(u+w)n$	$-(vn+m)$	$(u-w)n$
4	$(wn-m)^2/2$	$(v-u)n$	$-(u+v)n$	$-(wn+m)$
5	$(un+m)^2/2$	$un-m$	$(v+w)n$	$(w-v)n$
6	$(vn+m)^2/2$	$(u-w)n$	$vn-m$	$(u+w)n$
7	$(wn+m)^2/2$	$(u+v)n$	$(v-u)n$	$wn-m$
8	$\{[(u+v+w)n-m]/2\}^2$	$(v-u-w)n-m$	$(w-u-v)n-m$	$(u-v-w)n-m$
9	$\{[(u+v-w)n+m]/2\}^2$	$(u-w-v)n-m$	$(u+v+w)n-m$	$(u-v+w)n+m$
10	$\{[(v-u+w)n+m]/2\}^2$	$(u+v-w)n+m$	$(v-u-w)n-m$	$(u+v+w)n-m$
11	$\{[(u-v+w)n+m]/2\}^2$	$(u+v+w)n-m$	$(v-u+w)n+m$	$(w-v-u)n-m$
12	$\{[(u+v+w)n+m]/2\}^2$	$(u+v-w)n-m$	$(v+w-u)n-m$	$(u-v+w)n-m$
13	$\{[(u+v-w)n-m]/2\}^2$	$-(u+v+w)n-m$	$(u-v+w)n-m$	$(u-v-w)n+m$
14	$\{[(-u+v+w)n-m]/2\}^2$	$(u-v+w)n-m$	$(u+v+w)n+m$	$(w-v-u)n+m$
15	$\{[(u-v+w)n-m]/2\}^2$	$(v-u+w)n-m$	$(w-u-v)n+m$	$-(u+v+w)n-m$
16	$(u+v)^2n^2/2$	$-(wn+m)$	$wn-m$	$(u-v)n$
17	$(u-v)^2n^2/2$	$wn-m$	$wn+m$	$-(v+u)n$
18	$(u+w)^2n^2/2$	$vn-m$	$(w-u)n$	$-vn-m$
19	$(v+w)^2n^2/2$	$(v-w)n$	$-(un+m)$	$un-m$
20	$(u-w)^2n^2/2$	$(vn+m)$	$-(u+w)n$	$vn-m$
21	$(v-w)^2n^2/2$	$-(w+v)n$	$un-m$	$un+m$
22	u^2n^2	$-m$	wn	$-vn$
23	v^2n^2	$-wn$	$-m$	un
24	w^2n^2	vn	$-un$	$-m$

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

$(u-v)\alpha\Sigma$	$(2u-v-w)\alpha\Sigma$	$(u-2v-w)\alpha\Sigma$	$(u-v-2w)\alpha\Sigma$
$(u-w)\alpha\Sigma$	$(2u-v+w)\alpha\Sigma$	$(u-2v+w)\alpha\Sigma$	$(u-v+2w)\alpha\Sigma$
$(v-w)\alpha\Sigma$	$(2u+v-w)\alpha\Sigma$	$(u+2v-w)\alpha\Sigma$	$(u+v-2w)\alpha\Sigma$
$(u-v-w)\alpha\Sigma$	$(u-v+w)\alpha\Sigma$	$(u+v-w)\alpha\Sigma$	
$u\alpha\Sigma$	$v\alpha\Sigma$	$w\alpha\Sigma$	

cation, which appears for the first time, reduces the necessary library for every cubic CSL to only one piece of information, the smallest-angle description. All the other descriptions of this CSL are obtained from Table 1. Moreover, by inspection of Table 1, one can see some properties of the CSL considered. For example, if the smallest-angle description has two equal indices, it can be immediately seen from expressions 17, 20, 21 of Table 1 that there exists at least one 180° description for this CSL.

Let us now examine the DSCL construction. For a given CSL we know its symmetry by taking into account the theory established in paper I. Thus, from the corresponding Table 1 of this CSL, we can find a conventional base by making use of the symmetry axes. As a matter of fact the conventional unit cell and the primitive unit cell do not coincide for every Bravais lattice. But it is always possible to establish a relation between them and this is done for instance in Table 2.2.2 of Vol. I of *International Tables for X-ray Crystalllography* (1969). The procedure for the construction of the CSL* base will be shown analytically in a following example.

For the establishment of a general procedure, which could give the maximum information in a short time, we make use of Table 1 for every CSL and we take all the combinations of the different triplets, keeping the first axis invariant. We have computed these 253 combinations analytically and we give the smallest values of their determinants in Table 2.

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 Λ_1^1.

(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 $\Sigma = 13a$ CSL with smallest-angle description data

$$u=1;\ v=0;\ w=0;\ m=5;\ n=1;\ \alpha=2 \qquad (10)$$

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 $\Sigma = 13a$ CSL has tetragonal sym-

Table 3. *Symmetrically equivalent descriptions of $\Sigma = 13a$ CSL of the cubic system*

	ϑ	$[uvw]$		ϑ	$[uvw]$		ϑ	$[uvw]$
1	22·619	100	9	107·920	$\bar{2}\bar{2}3$	17	164·058	$\bar{5}5\bar{1}$
2	112·619	100	10	133·813	$3\bar{3}\bar{2}$	18	164·058	$\bar{5}1\bar{5}$
3	92·204	$\bar{1}51$	11	107.920	$\bar{2}2\bar{3}$	19	180.000	$0\bar{3}\bar{2}$
4	92·204	$\bar{1}1\bar{5}$	12	107.920	$\bar{2}3\bar{2}$	20	164.058	$5\bar{1}\bar{5}$
5	67·380	$\bar{1}00$	13	133·813	$3\bar{2}3$	21	180·000	$0\bar{2}3$
6	92·204	$1\bar{5}1$	14	107·920	$\bar{2}32$	22	157.380	$\bar{1}00$
7	92·204	$11\bar{5}$	15	133·813	$32\bar{3}$	23	180·000	$0\bar{5}1$
8	133·813	$33\bar{2}$	16	164·058	$\bar{5}5\bar{1}$	24	180·000	$01\bar{5}$

metry (see paper I). Thus, the triplets

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & \bar{2} & \bar{3} \\ 0 & 3 & \bar{2} \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 1 & 0 & 0 \\ 0 & \bar{5} & \bar{1} \\ 0 & 1 & \bar{5} \end{bmatrix} \tag{11}$$

have the symmetry properties, *i.e.* three mutually perpendicular vectors, two of them being 180° symmetry axes. Moreover, we can see that the determinant of the first matrix has a volume equal to 13 and, therefore, this is the convenient one for the CSL base computation. The second one has a volume equal to 26 and it can represent only a conventional base. By applying the smallest-angle rotation matrix R to the first matrix, we get

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & \bar{3} & \bar{2} \\ 0 & 2 & \bar{3} \end{bmatrix}, \tag{12}$$

which is the CSL base. By taking the inverse transpose of the previous matrix, which gives the product $\Sigma \times$ DSCL with the form

$$\begin{bmatrix} 13 & 0 & 0 \\ 0 & \bar{3} & \bar{2} \\ 0 & 2 & \bar{3} \end{bmatrix}, \tag{13}$$

the DSCL base can be obtained.

Finally, we should point out that our results have been compared with the results given by Grimmer *et al.* (1974). There is good agreement in almost all cases. The same type of vectors have been used, but they sometimes differ in the orientation. It can be easily deduced that these differences do not have any influence on the results obtained, and this is because they are looking for a numerical solution of the system (2) and from this the Bravais class is defined by the method described by Mighell, Santoro & Donnay in *International Tables for X-ray Crystallography* (1969).

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

Table 4. *Angles and rotation-axis indices of the different descriptions of the hexagonal CSLs*

	$4\alpha\Sigma \cos^2(\theta/2)$	u_r	v_r	w_r
1	$12\mu m^2$	u	v	w
2	$9\mu m^2+\mu wn[wn-6m]$	$2(2u-v)n$	$2(u+v)n$	$3(m+wn)$
3	$3\mu m^2+3\mu wn[wn-2m]$	$2(u-v)n$	$2un$	$3m+wn$
4	$3\mu m^2+3\mu wn[wn+2m]$	$-2vn$	$2(u-v)n$	$3m-wn$
5	$9\mu m^2+\mu wn[wn+6m]$	$-2(u+v)n$	$2(u-2v)n$	$3(m-wn)$
6	$(2u-v)^2\nu n^2$	$2(3m-wn)\mu$	$-4w\mu n$	$3v\nu n$
7	$(u-2v)^2\nu n^2$	$-4w\mu n$	$-2(3m+wn)\mu$	$3u\nu n$
8	$(u+v)^2\nu n^2$	$-2(3m+wn)\mu$	$2(-3m+wn)\mu$	$3(u-v)\nu n$
9	$3(u-v)^2\nu n^2$	$2(m-wn)\mu$	$-2(m+wn)\mu$	$(u+v)\nu n$
10	$3u^2\nu n^2$	$-4m\mu$	$2(-m+wn)\mu$	$(u-2v)\nu n$
11	$3v^2\nu n^2$	$-2(m+wn)\mu$	$-4m\mu$	$(2u-v)\nu n$
12	$4\mu w^2 n^2$	$(u-2v)n$	$(2u-v)n$	$3m$

(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 μ and ν, 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

$$R_j = g_j R, \qquad j = 1, 2, \ldots, 12. \tag{14}$$

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, w, m, n, α, μ, ν may have.

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

$$R^* = (1/\Sigma)[r_{ij}^*/\alpha]; \tag{15}$$

Table 5. *Rotation-axis indices of the different descriptions of the hexagonal CSLs in the reciprocal space*

	u_r^*	v_r^*	w_r^*
1	$(2u-v)\nu$	$(2v-u)\nu$	$2w\mu$
2	$(u-v)\nu n$	$v\nu n$	$(m+wn)\mu$
3	$(u-2v)\nu n$	$(u+v)\nu n$	$(3m+wn)\mu$
4	$-v\nu n$	$u\nu n$	$2m\mu$
5	$-(u+v)\nu n$	$(2u-v)\nu n$	$(3m-wn)\mu$
6	$-u\nu n$	$(u-v)\nu n$	$(m-wn)\mu$
7	$-2wn$	$wn-3m$	$(2u-v)n$
8	$-(3m+wn)$	$2wn$	$(u-2v)n$
9	$3m-wn$	$-(3m+wn)$	$(u+v)n$
10	$2m$	$-(wn+m)$	vn
11	$m-wn$	$-2m$	un
12	$-(wn+m)$	$wn-m$	$(u-v)n$

and the integer expressions r_{ij}^* have the following forms:

$$\begin{aligned}
r_{11}^* &= (2u-v)u\nu n^2 - 2w\mu mn + 3\mu m^2 - dn^2 \\
r_{12}^* &= (2u-v)v\nu n^2 - 4w\mu mn \\
r_{13}^* &= [(2u-v)wn^2 + 3vmn]\nu \\
r_{21}^* &= (2v-u)u\nu n^2 + 4w\mu mn \\
r_{22}^* &= (2v-u)v\nu n^2 + 2w\mu mn + 3\mu m^2 - dn^2 \\
r_{23}^* &= [(2v-u)wn^2 - 3umn]\nu \\
r_{31}^* &= [2uwn^2 + 2(u-2v)mn]\mu \\
r_{32}^* &= [2vwn^2 + 2(2u-v)mn]\mu \\
r_{33}^* &= 2w^2\mu n^2 + 3\mu m^2 - dn^2
\end{aligned} \tag{16}$$

and

$$d = (u^2 + v^2 - uv)\nu + \mu w^2, \tag{17}$$

where u, v, w, m, n, α, μ, ν are the integer numbers describing the given CSL in the direct space. The different rotation axes $\mathbf{r}_j^*, j = 1, 2, \ldots, 12$, 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 α are variable depending on the μ, ν values, the α 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 $\nu \equiv 0 \bmod 2$, the vectors $\mathbf{r}_1^*$, $\mathbf{r}_4^*$ have even indices.

(ii) If $\alpha = 4$ and $\nu \not\equiv 0 \bmod 2$, then

$$u \equiv 0 \bmod 2,\ v \equiv 0 \bmod 2,\ w \equiv 1 \bmod 2$$

$$m \equiv 1 \bmod 2,\ n \equiv 1 \bmod 2$$

and the indices of all the $\mathbf{r}_{ij}^*$ vectors are even numbers.

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

$\nu(2u-v)\alpha\Sigma$	$\nu(u-v)\alpha\Sigma$	$\nu v\alpha\Sigma$
$\nu(u-2v)\alpha\Sigma$	$2w\alpha\Sigma$	$\nu u\alpha\Sigma$

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

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

$$u + v \equiv 0 \bmod 3,\ w \equiv 0 \bmod 3,\ (u, v) \div 1$$

and

$$2u - v \equiv 0 \bmod 3,\ 2v - u \equiv 0 \bmod 3.$$

In this case the vectors $\mathbf{r}_1^*$, $\mathbf{r}_3^*$, $\mathbf{r}_5^*$, $\mathbf{r}_7^*$, $\mathbf{r}_8^*$, $\mathbf{r}_9^*$ have indices that are multiples of 3.

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

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

or

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

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

(iii) If $(m, d) \div t (t \neq 1)$, then there are again two possibilties: firstly, $t = 2$ and $\mu \equiv 0 \bmod 2$ and, secondly, $t \neq 2$ and $w \equiv 0 \bmod t$. For the first case the parameter α can be eliminated from the first six vectors, and for the second case we have $\nu \equiv 0 \bmod t$ and α is eliminated from the $\mathbf{r}_1^*$ vector.

(iv) If $(3, n) \div 3$, α is eliminated from the vectors $\mathbf{r}_7^*$, $\mathbf{r}_8^*$, $\mathbf{r}_9^*$.

(v) If $(\mu, n) \div p (p \neq 1)$, α 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 μ/ν 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 $(\mathbf{r}_1^*, \mathbf{r}_8^*, \mathbf{r}_{11}^*)$ and $(\mathbf{r}_1^*, \mathbf{r}_{10}^*, \mathbf{r}_{11}^*)$ give determinants with values

$$\begin{aligned}
\det[(\mathbf{r}_1^*), (\mathbf{r}_8^*), (\mathbf{r}_{11}^*)] &= 4w\alpha\Sigma = 4 \times 1 \times 96 \times 13 \\
&= 4992 \\
\det[(\mathbf{r}_1^*), (\mathbf{r}_{10}^*), (\mathbf{r}_{11}^*)] &= -2w\alpha\Sigma = -2 \times 1 \times 96 \times 13 \\
&= -2496.
\end{aligned}$$

The coordinates of these vectors are obtained from Table 5:

$$\mathbf{r}_1^*: (0, 0, 16)$$
$$\mathbf{r}_8^*: (\bar{24}, 6, 0)$$
$$\mathbf{r}_{10}^*: (14, \bar{10}, 0)$$
$$\mathbf{r}_{11}^*: (4, \bar{14}, 0).$$

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

$$B_1^* = \begin{bmatrix} 0 & \bar{4} & 2 \\ 0 & 1 & \bar{7} \\ 1 & 0 & 0 \end{bmatrix}, \qquad B_2^* = \begin{bmatrix} 0 & 7 & 2 \\ 0 & \bar{5} & \bar{7} \\ 1 & 0 & 0 \end{bmatrix},$$

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:

$$B_1^* = \begin{bmatrix} 0 & \bar{4}\times 5 + 3 \times 7 & 2 \\ 0 & 1 \times 5 + 3 \times \bar{5} & \bar{7} \\ 1 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 2 \\ 0 & \bar{10} & \bar{7} \\ 1 & 0 & 0 \end{bmatrix}$$

with $\det[B_1^*] = 13$ and

$$B_2^* = \begin{bmatrix} 0 & \bar{4}\times 2 + 1 \times 7 & 2 \\ 0 & 1 \times 2 + 1 \times \bar{5} & \bar{7} \\ 1 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & \bar{1} & 2 \\ 0 & \bar{3} & \bar{7} \\ 1 & 0 & 0 \end{bmatrix}.$$

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

$$R^* B_2^* = \frac{1}{13} \begin{bmatrix} 8 & \bar{7} & 0 \\ 7 & 15 & 0 \\ 0 & 0 & 13 \end{bmatrix} \begin{bmatrix} 0 & \bar{1} & 2 \\ 0 & \bar{3} & \bar{7} \\ 1 & 0 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 1 & 5 \\ 0 & \bar{4} & \bar{7} \\ 1 & 0 & 0 \end{bmatrix}.$$

By taking the inverse transpose of the previous matrix, which gives the product $\Sigma \times$DSCL with the form

$$\begin{bmatrix} 0 & \bar{7} & 4 \\ 0 & \bar{5} & 1 \\ 13 & 0 & 0 \end{bmatrix},$$

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, α and μ, ν, 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 crystallograhic 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 μ/ν 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

BLERIS, G. L. (1983). *Phys. Status Solidi A*, **75**, K83-K85.

BLERIS, G. L. & DELAVIGNETTE, P. (1981). *Acta Cryst.* A**37**, 779-786.

BLERIS, G. L., NOUET, G., HAGÈGE, S. & DELAVIGNETTE, P. (1982). *Acta Cryst.* A**38**, 550-557.

BOLLMANN, W. (1970). *Crystal Defects and Crystalline Interfaces.* Berlin: Springer-Verlag.

BONNET, R. (1976). *Scr. Metall.* **10**, 801-803.

BONNET, R., COUSINEAU, E. & WARRINGTON, D. H. (1981). *Acta Cryst.* A**37**, 184-189.

BONNET, R. & DURAND, F. (1975). *Scr. Metall.* **9**, 935-939.

DONI, E. G., BLERIS, G. L., KARAKOSTAS, TH., ANTONOPOULOS, J. G. & DELAVIGNETTE, P. (1985). *Acta Cryst.* A**41**, 440-445.

FORTES, M. A. (1983). *Acta Cryst.* A**39**, 351-357.

GRIMMER, H. (1974). *Scr. Metall.* **8**, 1221-1223.

GRIMMER, H., BOLLMANN, W. & WARRINGTON, D. H. (1974). *Acta Cryst.* A30, 197-207.
GRIMMER, H. & WARRINGTON, D. H. (1983). *Z. Kristallogr.* 162, 88-90.
HAGÈGE, S., NOUET, G. & DELAVIGNETTE, P. (1980). *Phys. Status Solidi A*, 62, 97-107.
International Tables for X-ray Crystallography (1969). Vol. I. Birmingham: Kynoch Press.
KARAKOSTAS, TH., BLERIS, G. L. & ANTONOPOULOS, J. G. (1979). *Phys. Status Solidi A*, 55, 801-809.
KARAKOSTAS, TH., NOUET, G. & DELAVIGNETTE, P. (1979). *Phys. Status Solidi A*, 52, 65-76.

Acta Cryst. (1985). A41, 451-453

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

BY J. Z. TISCHLER

Oak Ridge National Laboratory, Solid State Division, Oak Ridge, Tennessee 37831, *USA*

AND Q. SHEN AND R. COLELLA

Purdue University, Department of Physics, West Lafayette, Indiana 47907, *USA*

(*Received* 27 *December* 1984; *accepted* 4 *April* 1985)

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 θ, 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 φ, the azimuthal angle around the scattering vector, in such a way as to keep the excitation weak. In a plot of R_θ^{hkl} *vs* φ, R_θ^{hkl} being the integrated intensity of the *hkl* reflection integrated with respect to θ at constant φ, 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

* Since silicon is centrosymmetric, all phases, including those of forbidden reflections, are 0 or π.

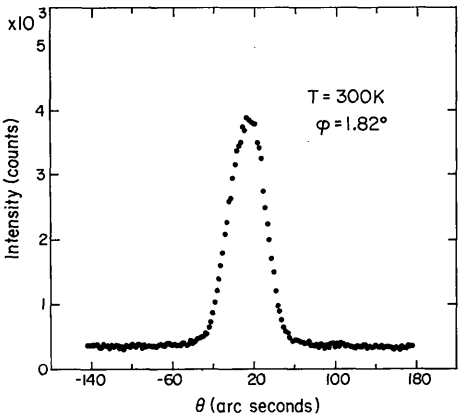

Fig. 1. Typical 442 rocking curve at $T = 300$ K. The zero on the θ scale is arbitrary. Intensity values are referred to a monitor count of 2×10^5, and the average counting time per point is approximately 3 s. At this φ value the 442 is about three times greater than the two-beam value, owing to perturbation effects introduced by the strong $\bar{1}1\bar{1}$ *Umweganregung* peak, centered at about $\varphi = 3{\cdot}00°$.

0108-7673/85/050451-03$01.50