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Computation of Coincident and Near-Coincident Cells for Any Two Lattices – Related DSC-1 and DSC-2 Lattices

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A computation method is presented for determining: (i) pairs of non-primitive cells $M1$ and $M2$, constructed on three translation vectors of a lattice 1 and three vectors of a lattice 2 respectively, such that the sizes of $M1$ and $M2$ are (almost) identical; (ii) Σ_1 (Σ_2), defined by the number of primitive cells of lattice 1 (lattice 2) contained in $M1$ ($M2$); (iii) a characteristic relative orientation of the two lattices for which $M1$ and $M2$ coincide exactly or approximately, for which the transformation relating $M1$ to $M2$ (denoted A in general) is a pure deformation, whose principal strains are calculated; (iv) base vectors for the DSC-1 and DSC-2 lattices, so that the Burgers vectors of intrinsic phase (or grain) boundary dislocations are determined. The DSC-1 lattice is constructed by summing the vectors of lattice 1 and lattice 2′, deduced from lattice 2 by A^{-1}. The DSC-2 lattice is derived from the DSC-1 lattice by A. Tables of results are presented for a lattice 1/lattice 2 of Zn/Zn, up to $\Sigma_1=\Sigma_2=25$, and for Ni_3Al (cubic)/Ni_3Nb (orthorhombic), up to $\Sigma_1=21$ and $\Sigma_2=10$.

1. Introduction

Although the geometrical conditions giving rise to the coincidence of two cells $M1$ and $M2$ belonging to two lattices 1 and 2 have been studied by several authors (see, for example, Friedel, 1964; Santoro & Mighell, 1973), complete calculations have only been performed for the cases of two identical cubic lattices (Grimmer, Bollmann & Warrington, 1974; Goux, 1974) and two identical hexagonal lattices with an ideal c/a ratio of $(8/3)^{1/2}$ (Fortes, 1973; Warrington, 1975). However, for hexagonal metals, these ratios can be markedly different and are never ideal in the cases of interest. Some cases of exact and near coincidence of two cells $M1$ and $M2$ have been calculated by Bruggemann, Bishop & Hartt (1972) for hexagonal lattices having different c/a ratios and by Bonnet & Durand (1975) for different lattices 1 and 2. In this work, it is shown how to calculate in the general case all the different pairs of cells $M1$ and $M2$ of any two lattices 1 and 2 such that $M1$ and $M2$ have almost (or exactly) the same size and how to determine a relative orientation of the lattices 1 and 2 which brings $M1$ and $M2$ into coincidence or near coincidence. $M1$ is defined uniquely as a Niggli reduced cell (Niggli, 1928; Křivý & Gruber, 1976). In particular, its base vectors $\mathbf{x}_i^1$ ($i=1,2,3$) obey the inequality

$$|\mathbf{x}_1^1|\le|\mathbf{x}_2^1|\le|\mathbf{x}_3^1| \tag{1}$$

while its three angular parameters are all less than or more than $\pi/2$. Correspondingly, $M2$ is a cell of lattice 2, with base vectors $\mathbf{x}_i^2$ ($i=1,2,3$), which can be superposed on cell $M1$ within a given tolerance. The cell $M2$ may or may not be a Niggli reduced cell. For instance, the angular parameters of $M2$ may deviate slightly from those of $M1$ without being necessarily all acute or obtuse as required for $M1$. In this work, a pair of cells $M1$ and $M2$ is said to be 'different' from a pair of cells $M1'$ and $M2'$ if the sizes of $M1$ and $M2$ cannot be exactly superposed on $M1'$ and $M2'$ respectively. Otherwise, the two pairs of cells are said to be 'identical'.

Two examples are shown to illustrate the computational method proposed. They give results concerning the cells $M1$ and $M2$ occurring in the twin orientations of Zn and in the eutectic alloy Ni_3Al(cubic)/Ni_3Nb(orthorhombic). Other results are derived, in particular, base vectors for the DSC-1 and DSC-2 lattices (Bonnet & Durand, 1975) which define the possible Burgers vectors of intrinsic phase- (or grain-) boundary dislocations. These lattices extend the concept of the DSC lattices introduced by Bollmann (1967, 1970) and Warrington & Bollmann (1972) in the cases where $M1$ and $M2$ are exactly the same size.

2. Analytical relations corresponding to a near coincidence of two cells M1 and M2

The orientations of lattices 1 and 2 are referred to an orthonormal frame $F0$ of base vectors $\mathbf{e}_i$ ($i=1,2,3$). The three base vectors $\mathbf{a}_i^1$ (frame $F1$) of a primitive cell of lattice 1, hereinafter considered to be fixed in space, are defined by the transformation S_1:

$$(\mathbf{a}_i^1)=S_1(\mathbf{e}_i)\,. \tag{2}$$

The initial orientation of a primitive cell $\mathbf{a}_i^2$ (frame $F2$) of lattice 2 is determined by the three vectors $\mathbf{a}_i^{2,0}$, known from a given transformation $S_{2,0}$:

$$(\mathbf{a}_i^{2,0})=S_{2,0}(\mathbf{e}_i)\,. \tag{3}$$

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The frames $F0$, $F1$, $F2$, are taken with a common origin.

Now let us assume that lattice 2 undergoes a rotation described by a vector $\mathbf{R}$ (components p, q, r in $F0$). The vector $\mathbf{R}$ is parallel to the rotation axis, $|\mathbf{R}|$ being the rotation angle. The sense of $\mathbf{R}$ defines a right-handed screw rotation. R and V are two transformations related to the rotation of lattice 2:

$$(\mathbf{a}_i^2)=\mathsf{R}(\mathbf{a}_i^{2,0}) \tag{4}$$

$$(\mathbf{a}_i^2)=\mathsf{V}(\mathbf{a}_i^1)\,. \tag{5}$$

R is supposed to be such that two cells $M1$ and $M2$ are in exact or near coincidence. Fig. 2 of Bonnet & Durand (1975) describes the situation. The base vectors of the cells $M1$ and $M2$, denoted $\mathbf{x}_i^1$ and $\mathbf{x}_i^2$ respectively, are defined from the vectors $\mathbf{a}_i^1$ and $\mathbf{a}_i^2$ by the transformations U_1 and U_2:

$$(\mathbf{x}_i^1)=\mathsf{U}_1(\mathbf{a}_i^1) \tag{6}$$

$$(\mathbf{x}_i^2)=\mathsf{U}_2(\mathbf{a}_i^2)\,. \tag{7}$$

Expressed in the frames $F1$ and $F2$, these two transformations are integer matrices. The determinants of U_1 and U_2 define respectively the integers Σ_1 and Σ_2.

We introduce now some quantities useful for the analysis: a transformation A relating $M1$ to $M2$, and a third lattice, the lattice 2′. A is defined by:

$$(\mathbf{x}_i^2)=\mathsf{A}(\mathbf{x}_i^1) \quad (i=1,2,3)\,. \tag{8}$$

The principal strains ε_1, ε_2, ε_3, of the pure deformation D relating $M1$ to $M2$ can be calculated from A by the following equation (Bonnet & Durand, 1975*a*):

$$\mathsf{A}=\mathsf{R}_p\mathsf{D} \tag{9}$$

where R_p is a pure rotation.

The transformation A, close to the identity transformation, allows us to define the lattice 2′ (base vectors $\mathbf{a}_i^{2\prime}$, frame $F2'$) which differs only slightly from the lattice 2. Following Bonnet (1974) and Bonnet & Durand (1975*a*):

$$(\mathbf{a}_i^{2\prime})=\mathsf{A}^{-1}(\mathbf{a}_i^2)\,. \tag{10}$$

Combining (8) and (10) shows that for any A transformation the cell $M1$ is exactly common to both lattices 1 and 2′. The base vectors of $M1$ can also be defined from the vectors $\mathbf{a}_i^{2\prime}$ by the transformation U_2':

$$(\mathbf{x}_i^1)=U_2'(\mathbf{a}_i^{2\prime})\,. \tag{11}$$

Expressed in the frame $F2'$, this transformation is an integer matrix. The vectors $\mathbf{a}_i^{2\prime}$ are related to the vectors $\mathbf{a}_i^1$ by a transformation U:

$$(\mathbf{a}_i^{2\prime})=\mathsf{U}(\mathbf{a}_i^1)\,. \tag{12}$$

U is of importance later in the analysis to find base vectors for the DSC-1 lattice, defined by summing the translation vectors of lattices 1 and 2′. The DSC-2 lattice is deduced from the DSC-1 lattice by the transformation A.

Fig. 1 defines the transformations which relate the several base vectors and reference frames $F0$, $F1$, $F2$, $F2'$ used. From Fig. 1 and matrix algebra we can express the transformations V and U_1 in the frame $F1$ and the transformation U_2 in the frame $F2$:

$$[\mathsf{V}]_{F1}=[\mathsf{S}_1^{-1}]_{F0}[\mathsf{R}]_{F0}[\mathsf{S}_{2,0}]_{F0} \tag{13}$$

$$[\mathsf{V}]_{F1}=[\mathsf{A}]_{F1}[\mathsf{U}]_{F1} \tag{14}$$

$$[\mathsf{U}_1]_{F1}=[\mathsf{U}]_{F1}[\mathsf{U}_2']_{F2'} \tag{15}$$

$$[\mathsf{U}_2]_{F2}=[\mathsf{U}_2']_{F2'} \tag{16}$$

where $[\mathsf{R}]_{F0}$ is the rotation matrix expressed in $F0$, related to the rotation vector $\mathbf{R}$. Equation (13) gives the elements of $[\mathsf{V}]_{F1}$ once $[\mathsf{R}]_{F0}$ is obtained from the three components p, q, r of $\mathbf{R}$. In equation (15), the matrices $[\mathsf{U}_1]_{F1}$ and $[\mathsf{U}_2']_{F2'}$ have integer elements so that the matrix $[\mathsf{U}]_{F1}$ is a rational matrix. Since $[\mathsf{A}]_{F1}$ is close or equal to the identity matrix, equation (14) shows that the elements of the matrix $[\mathsf{V}]_{F1}$ are close or equal to the rational elements of $[\mathsf{U}]_{F1}$. These latter can be written from equation (15), u_{ij}/Σ_2 or u_{ij}'/N, where N is the lowest common denominator of the fractions u_{ij}/Σ_2. Writing v_{ij} for the elements of $[\mathsf{V}]_{F1}$, it follows from equation (14) that the integers u_{ij} may be found from the numbers obtained from (Nv_{ij}) rounded to the nearest integer, *i.e.*

$$u_{ij}'=\mathrm{ROUND}\,(Nv_{ij})\,. \tag{17}$$

The slight mismatch of $M1$ and $M2$ may thus be characterized by the nine small numbers $|u_{ij}'-Nv_{ij}|$. We seek $M1$ and $M2$ in which these nine numbers are all smaller than a given value Δu, obviously less than 0·5:

$$u_{ij}'-Nv_{ij}<\Delta u\,. \tag{18}$$

The problem of finding the pairs of cells $M1$ and $M2$ has now been reduced to the following: for $1\le N\le\Sigma_{2\,\max}$ find the rotation $\mathbf{R}(p,q,r)$ so that the elements of $[\mathsf{V}]_{F1}$ satisfy the inequalities (18). Then, using the matrix $[\mathsf{U}]_{F1}$ according to Bonnet (1976), determine a unit cell of the coincidence site lattice

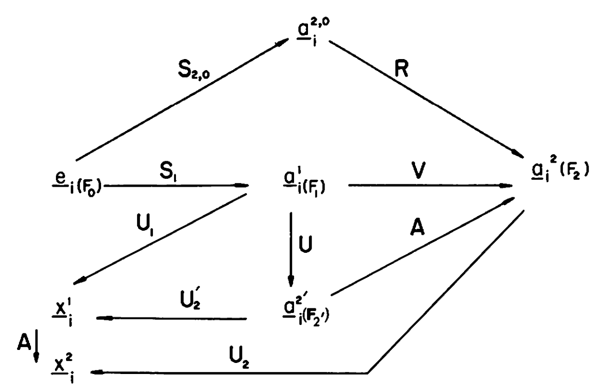

Fig. 1. Definition of the transformations (S_1, V, *etc.*) relating the different bases ($\mathbf{a}_i^1$, $\mathbf{e}_i$, *etc.*). The bases $\mathbf{e}_i$, $\mathbf{a}_i^1$, $\mathbf{a}_i^2$, $\mathbf{a}_i^{2\prime}$ define the reference frames $F0$, $F1$, $F2$, $F2'$ respectively.

(CSL) between lattices 1 and 2′. Finally, applying a reduction procedure, find the $M1$ cell and then the $M2$ cell by applying equations (15) and (16).

3. Determination of R

Since any small variations of p, q, r can maintain $M1$ and $M2$ in near coincidence, it is necessary to define more precisely the rotation **R** to be computed. Let us now suppose that lattice 2 undergoes rotations **R** such that a vector $\mathbf{V}^2$ of lattice 2 remains parallel or antiparallel to a vector $\mathbf{V}^1$ of lattice 1, the lengths $|\mathbf{V}^1|$ and $|\mathbf{V}^2|$ differing only by a small length ΔL. Vectors $\mathbf{V}^1$ and $\mathbf{V}^2$ obey the relations:

$$\mathbf{V}^1 \| \mathbf{V}^2 \tag{19}$$

or

$$\mathbf{V}^1 \| -\mathbf{V}^2 \tag{20}$$

$$||\mathbf{V}^2|-|\mathbf{V}^1|| < \Delta L\,. \tag{21}$$

In this work, the above relations are used to seek the pairs of cells $M1$ and $M2$. To limit the number of possible vectors $\mathbf{V}^1$ and $\mathbf{V}^2$ obeying the inequalities (21), a maximum value is now chosen for the volume of the cell $M1$, *i.e.* Σ_1 is chosen less than or equal to $\Sigma_{1\ \max}$. The Appendix shows that the vectors $\mathbf{x}_1^1$ of all the cells $M1$ obey the following inequality:

$$|\mathbf{x}_1^1| \le (v_1 \Sigma_{1\ \max})^{1/3} 2^{1/6} = L \tag{22}$$

where v_1 is the volume of a primitive cell of lattice 1. Consequently, looking for all the vectors $\mathbf{V}^1$ such that:

$$|\mathbf{V}^1| \le L \tag{23}$$

enables the computer calculation to arrive at an axis defined by the smallest vector of each cell $M1$. From the inequalities (21) and (23), we deduce a limitation on the length of vectors $\mathbf{V}^2$:

$$|\mathbf{V}^2| \le L + \Delta L \tag{24}$$

and accordingly a limitation on the number of vectors $\mathbf{V}^2$.

The maximum value for Σ_2, denoted $\Sigma_{2\ \max}$, is needed in (18) to limit the search for the matrices $[\mathsf{U}]_{F1}$. $\Sigma_{2\ \max}$ and is derived from $\Sigma_{1\ \max}$ and (8):

$$\Sigma_{2\ \max} = v_1\, \Sigma_{1\ \max} \det \mathsf{A} / v_2 \tag{25}$$

where det A is the determinant of A. Noting that the sum

$$S = |\varepsilon_1| + |\varepsilon_2| + |\varepsilon_3| \tag{26}$$

is small and that [equation (9)] det A may be expressed to a first order

$$\det \mathsf{A} = 1 + \varepsilon_1 + \varepsilon_2 + \varepsilon_3\,, \tag{27}$$

we deduce the following inequality:

$$\Sigma_{2\ \max} \le v_1\, \Sigma_{1\ \max}(1+S)/v_2\,. \tag{28}$$

In this work, S is chosen less than an arbitrary value S max:

$$S < S \max\,. \tag{29}$$

Calling INT the function which truncates at the decimal point we derive $\Sigma_{2\ \max}$ as:

$$\Sigma_{2\ \max} = \mathrm{INT}[v_1\, \Sigma_{1\ \max}(1 + S \max)/v_2]\,. \tag{30}$$

The number of vectors $\mathbf{V}^1$ and $\mathbf{V}^2$ to be computed may be considerably reduced if the symmetries of the lattices are taken into account, for the following reasons: (1) the higher the symmetry of the lattices 1 and 2, the lower are the number of different forms of vectors $\mathbf{V}^1$ and $\mathbf{V}^2$ to be kept in respect of the relations (21), (23) and (24); (2) if a binary axis of lattice 1 (lattice 2) is perpendicular to $\mathbf{V}^1$ ($\mathbf{V}^2$), the relation (20) will give identical pairs of cells $M1$ and $M2$; (3) if either $\mathbf{V}^1$ or $\mathbf{V}^2$ is a symmetry axis of order n, the rotation θ around $\mathbf{V}^1$ may be reduced to $2\pi/n$, (4) if the greatest common divisor of the components of $|\mathbf{V}^1|_{F1}$ and $|\mathbf{V}^2|_{F2}$ is an integer n greater than 1, the vectors $\mathbf{V}^1$ and $\mathbf{V}^2$ are to be rejected because the direction $\mathbf{V}^1 \| \mathbf{V}^2$ is also defined by the relation $\mathbf{V}^1/n \| \mathbf{V}^2/n$; (5) if the lattices are the same, rotations of lattice 2 around $\mathbf{V}^1 \| \mathbf{V}^2$ will lead to the same pairs of cells $M1$ and $M2$ as rotations around $\mathbf{W}^1 \| \mathbf{W}^2$ where $\mathbf{W}^1$ and $\mathbf{W}^2$ have the same form as $\mathbf{V}^2$ and $\mathbf{V}^1$ respectively. In addition, a pair of cells $M1$ and $M2$ and a pair of cell $M1'$ and $M2'$ may be considered identical if $M1$ and $M2$ can be superposed respectively on $M2'$ and $M1'$.

4. Algorithm (Fig. 2)

The matrix $[\mathsf{R}]_{F0}$, which depends on θ, can be expressed by the product

$$[\mathsf{R}(\theta)]_{F0} = [\mathsf{R}_2(\theta)]_{F0}[\mathsf{R}_1]_{F0}\,. \tag{31}$$

First, the rotation R_1 turns lattice 2 from its initial orientation into an orientation such that $\mathbf{V}^2$ becomes parallel or antiparallel to $\mathbf{V}^1$. Second, lattice 2 is turned by the rotation $\mathsf{R}_2(\theta)$ whose axis is parallel to $\mathbf{V}^1$. Third, the angle θ is increased in small increments $\Delta\theta$. For each value of θ and $N(\le \Sigma_{2\ \max})$, the computer calculates successively the matrices $[\mathsf{R}(\theta)]_{F0}$ by equation (31), $[\mathbf{V}]_{F1}$ by equation (13), $[\mathsf{U}]_{F1}$ by equation (17). If the inequality (18) is satisfied, the computer determines, using only $[\mathsf{U}]_{F1}$, the quantities Σ_1, Σ_2 and a unit cell for the CSL defined by the lattice 1 and 2′ (Bonnet, 1976).* Then, using an algorithm based on the works of Buerger (1957, 1960), and Balashov & Ursell (1957), the computer determines the cell $M1$, *i.e.* $[\mathsf{U}_1]_{F1}$. The cell $M2$ is determined by $[\mathsf{U}_2]_{F2}$ from (15) and (16). Finally, the pair of cells $M1$ and $M2$ is compared with each of the previously obtained pairs. Finding a new pair of cells $M1$ and $M2$ different from all the other pairs of cells previously found causes the computer to store Σ_1, Σ_2, and

* In this paper, the inequality line 19 on p. 802 must be written $0 \le \beta\mu/\Sigma_2 < 1/\lambda$, as noted by H. Grimmer (private communication).

$[A]_{F0}$. $[A]_{F0}$ is calculated from the following expression, deduced from (14) with matrix calculation:

$$[A]_{F0}=[S_1]_{F0}[V]_{F1}[U^{-1}]_{F1}[S_1^{-1}]_{F0}. \quad (32)$$

The computer also stores the components p, q, r of the rotation vector **R**, in $F0$.

It is worth noting here that other rotation vectors (called **R**′), not stored by the computer, may exist, which lead to pairs of cells $M1'$ and $M2'$, identical with $M1$ and $M2$, but not necessarily to the same DSC-1 and DSC-2 lattices.

We may write the transformation R′ as a product:

$$(R')=(X)(R). \quad (33)$$

If $(X)=(R_1')(R_2')$, [or $(R_2')(R_1')$] where the rotations R_1', R_2', are symmetry operations for lattices 1 and 2 respectively, then the DSC-1 and DSC-2 lattices are unchanged. In other cases, new DSC-1 and DSC-2 lattices will in general be found for R′. In such cases, the rotation (X) may bring $M2$ into near coincidence with $M1'$. In this case, we must have an exact CSL between two identical lattices 1, for which $\Sigma=\Sigma_1$. Or, (X) may bring a cell $M2'$ into near coincidence with $M1$. In this case, there must exist an exact CSL between two identical lattices 2, for which $\Sigma=\Sigma_2$. Finally, (X) may bring a cell $M^{2'}$ into near coincidence with $M1'$. In this case, CSL's must exist for identical lattices 1 and 2 respectively with multiplicities Σ_1 and Σ_2.

Having stored Σ_1, Σ_2, $[A]_{F0}$ and **R** (p, q, r) the computer then determines: (1) base vectors for a first unit cell of the DSC-1 lattice, derived from $[U]_{F1}$ following Bonnet (1976); (2) by reduction of this first unit cell, a Niggli reduced cell of the DSC-1 lattice; (3) a unit cell for the DSC-2 lattice by applying the transformation A to the Niggli reduced cell of the DSC-1 lattice; (4) the components of the eigenvectors of the pure deformation D relating $M1$ to $M2$ and the principal strains $\varepsilon_1, \varepsilon_2, \varepsilon_3$ [see equations (11) and (13) of Bonnet & Durand (1975*a*)]; the cells $M1$ and $M2$ for which $S \geq S$ max are not retained; (5) the orientation of lattice 2 such that the new transformation relating $M1$ to $M2$ is a pure deformation. This orientation, determined by the rotation vector $\mathbf{R}_d$ (components r_1, r_2, r_3 in $F0$), is calculated from $[R]_{F0}$ and (9).

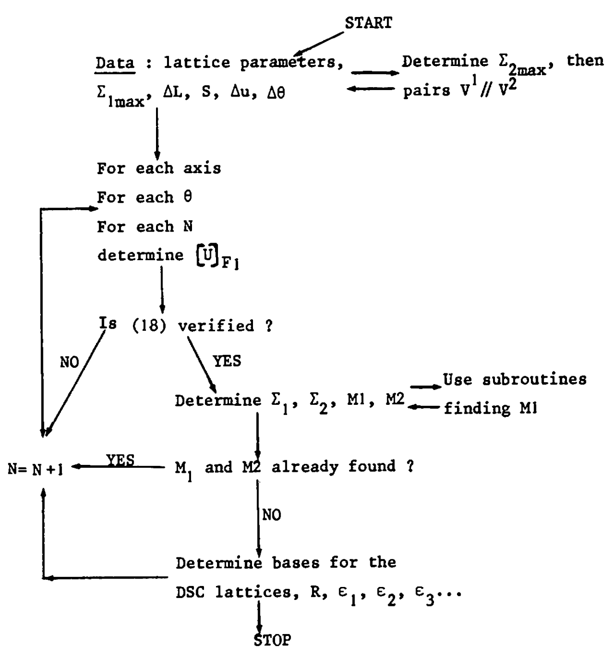

Fig. 2. Simplified flow chart of the computer program.

5. Example 1: Ni_3Al/Ni_3Nb (Table 1)

For simplicity, the lattices of Ni_3Al and Ni_3Nb are respectively denoted lattice 1 and lattice 2. The parameters of the Ni_3Al (cubic) and Ni_3Nb (orthorhombic) primitive cells are taken as those measured in the eutectic Ni_3Al–Ni_3Nb. For Ni_3Al, $a=3{\cdot}592$ Å

Table 1. *Near-coincident cells for lattice* 1 (Ni_3Al, *cubic*) *and lattice* 2 (Ni_3Nb, *orthorhombic*) *and other related crystallographic quantities. Computation performed for* $\Sigma_{1\,max}=21$, $\Delta L=0{\cdot}5$ Å, $S_{max}=0{\cdot}102$, $\Delta u=0{\cdot}4$, $\Delta\theta=0{\cdot}003$ rad

Σ_1	Σ_2	M1 $[U_1]_{F_1}$	M2 $[U_2]_{F_2}$	Sym M1	ε_1 ε_2 ε_3	R_d {r_1 r_2 r_3 (rd) $\lvert R_d\rvert$	N	$[U]_{F_1}$ (×N)	$[DSC1]_{F_1}$ ×Σ_2	$[DSC2]_{F_2}$ ×Σ_1
10 (12) (16) (18)	5 (6) (7) (9)	$\bar{1}\ \bar{1}\ \bar{2}$ $1\ \bar{1}\ \bar{2}$ $0\ \bar{1}\ 3$	$\bar{1}\ 0\ 0$ $0\ \bar{1}\ \bar{3}$ $0\ \bar{1}\ 2$	mo P	-0.006 0.005 0.052	-0.193 0.080 -0.783 0.810	5	$5\ 4\ 1$ $\bar{5}\ 4\ 1$ $0\ \bar{1}\ 6$	$1\ \bar{2}\ 3$ $1\ \bar{2}\ \bar{2}$ $1\ 3\ \bar{2}$	$0\ 0\ 5$ $2\ \bar{6}\ 2$ $2\ 4\ \bar{3}$
12 (16)	6 (8)	$\bar{1}\ 1\ 2$ $1\ 1\ 2$ $0\ 2\ \bar{2}$	$\bar{1}\ 0\ 0$ $0\ 0\ 3$ $0\ 2\ 0$	or P	0.005 0.019 0.027	-0.583 0.242 -0.760 0.988	6	$6\ 4\ 3$ $\bar{6}\ 4\ 3$ $0\ \bar{4}\ 6$	$1\ 2\ \bar{3}$ $1\ 2\ 3$ $2\ \bar{2}\ 0$	$0\ 0\ \bar{6}$ $0\ 6\ 0$ $4\ 0\ 0$
12	6	$1\ \bar{2}\ \bar{1}$ $\bar{1}\ \bar{2}\ \bar{1}$ $0\ 0\ \bar{3}$	$1\ 0\ 0$ $0\ \bar{1}\ \bar{3}$ $0\ 2\ 0$	mo P	-0.021 0.005 0.070	1.088 -0.451 -0.695 1.368	6	$6\ 2\ \bar{5}$ $\bar{6}\ 2\ \bar{5}$ $0\ 6\ 3$	$2\ 1\ 4$ $2\ 1\ \bar{2}$ $0\ 3\ 0$	$0\ 0\ 6$ $2\ 6\ 1$ $\bar{4}\ 0\ \bar{2}$
12 (14) (16)	6 (7) (8)	$\bar{1}\ 1\ 2$ $1\ 1\ 2$ $0\ 1\ \bar{4}$	$\bar{1}\ 0\ 0$ $0\ 1\ \bar{3}$ $0\ \bar{1}\ \bar{3}$	or P	-0.022 0.005 0.069	1.322 -0.548 -0.650 1.572	6	$6\ 1\ \bar{5}$ $\bar{6}\ 1\ \bar{5}$ $0\ 7\ 1$	$1\ \bar{2}\ \bar{4}$ $1\ 4\ 2$ $1\ \bar{2}\ 2$	$0\ \bar{6}\ \bar{6}$ $2\ \bar{3}\ 3$ $\bar{2}\ \bar{3}\ 3$
18	8	$1\ \bar{1}\ \bar{3}$ $\bar{1}\ \bar{1}\ \bar{3}$ $0\ 2\ \bar{3}$	$1\ 0\ 0$ $0\ \bar{2}\ 0$ $0\ 0\ \bar{4}$	or P	-0.039 -0.031 0.005	-0.904 0.375 -0.724 1.217	4	$4\ 2\ 3$ $\bar{4}\ 2\ 3$ $0\ \bar{4}\ 3$	$\bar{2}\ \bar{2}\ 4$ $\bar{2}\ \bar{2}\ \bar{4}$ $2\ \bar{2}\ 0$	$0\ 0\ 9$ $\bar{6}\ 0\ 0$ $\bar{2}\ 6\ 0$
18	9	$1\ 1\ \bar{3}$ $0\ \bar{1}\ \bar{6}$ $\bar{1}\ 1\ \bar{3}$	$1\ 0\ 0$ $0\ 1\ \bar{5}$ $0\ 1\ 4$	or P	-0.014 0.005 0.061	1.270 0.661 -0.526 1.526	9	$9\ 7\ 2$ $0\ 2\ \overline{11}$ $\bar{9}\ 7\ 2$	$1\ \bar{3}\ \bar{6}$ $\bar{1}\ 3\ \bar{3}$ $1\ 6\ 3$	$0\ \bar{9}\ \bar{9}$ $2\ 5\ \bar{5}$ $2\ \bar{4}\ 4$
19	9	$2\ 1\ 0$ $\bar{1}\ 2\ \bar{1}$ $0\ 2\ 3$	$1\ \bar{1}\ 1$ $1\ \bar{1}\ \bar{2}$ $1\ 2\ 1$	tri	-0.047 -0.005 0.050	-0.969 0.519 -1.307 1.707	3	$1\ 2\ 3$ $\bar{4}\ 0\ 1$ $1\ \bar{3}\ 2$	$3\ 0\ 0$ $0\ 3\ 6$ $0\ \bar{3}\ 3$	$1\ \bar{5}\ \bar{8}$ $3\ 4\ \bar{5}$ $4\ \bar{1}\ 6$
20	9	$\bar{1}\ \bar{2}\ \bar{1}$ $1\ \bar{2}\ \bar{1}$ $0\ 0\ 5$	$\bar{1}\ 0\ 0$ $0\ \bar{2}\ \bar{3}$ $0\ \bar{1}\ 3$	mo P	-0.057 -0.002 0.005	-0.465 0.193 0.769 0.919	9	$9\ 7\ 4$ $\bar{9}\ 7\ 4$ $0\ \bar{5}\ 10$	$1\ 3\ 5$ $1\ 3\ \bar{4}$ $\bar{2}\ 3\ \bar{1}$	$0\ 0\ 10$ $4\ 4\ 2$ $\bar{2}\ 8\ \bar{1}$
20	9	$\bar{1}\ 2\ 1$ $1\ 2\ 1$ $0\ 0\ \bar{5}$	$\bar{1}\ 0\ 0$ $0\ 2\ \bar{1}$ $0\ \bar{1}\ \bar{4}$	mo P	-0.057 -0.002 0.005	0.465 -0.193 -0.769 0.919	9	$9\ 7\ \bar{4}$ $\bar{9}\ 7\ \bar{4}$ $0\ 5\ 10$	$1\ 3\ \bar{4}$ $1\ 3\ 5$ $2\ \bar{3}\ 1$	$0\ 0\ \overline{10}$ $4\ 4\ 2$ $2\ \bar{8}\ 1$
20	10	$1\ \bar{1}\ \bar{3}$ $\bar{1}\ \bar{1}\ \bar{3}$ $0\ 3\ \bar{1}$	$1\ 0\ 0$ $0\ 2\ \bar{2}$ $0\ 2\ 3$	mo P	-0.006 0.005 0.052	1.150 -0.476 -0.684 1.421	10	$10\ 3\ \bar{8}$ $\overline{10}\ 3\ \bar{8}$ $0\ 11\ 4$	$\bar{1}\ 3\ \bar{6}$ $\bar{1}\ 3\ 4$ $3\ 1\ \bar{2}$	$0\ 0\ \overline{10}$ $4\ 4\ \bar{4}$ $4\ \bar{6}\ 1$
21	10	$2\ 1\ 2$ $\bar{1}\ 0\ 4$ $0\ \bar{2}\ 1$	$1\ 1\ \bar{2}$ $1\ 1\ 3$ $1\ \bar{1}\ 0$	mo P	-0.019 -0.006 0.027	0.156 0.627 -1.047 1.230	10	$5\ 10\ 5$ $\overline{11}\ 6\ \bar{5}$ $\bar{8}\ \bar{2}\ 10$	$0\ 0\ \bar{5}$ $\bar{2}\ 4\ \bar{1}$ $4\ 2\ 2$	$\bar{1}\ 6\ \bar{3}$ $\bar{3}\ 3\ \bar{9}$ $7\ 0\ 0$
21	10	$\bar{2}\ \bar{1}\ \bar{2}$ $1\ 0\ \bar{4}$ $0\ \bar{2}\ 1$	$\bar{1}\ \bar{1}\ \bar{2}$ $\bar{1}\ \bar{1}\ 3$ $\bar{1}\ 1\ 0$	mo P	-0.019 -0.006 0.027	2.578 0.372 0.496 2.651	10	$13\ 2\ 5$ $5\ \overline{10}\ \bar{5}$ $4\ 6\ \overline{10}$	$2\ \bar{4}\ 1$ $0\ 0\ 5$ $\bar{4}\ \bar{2}\ \bar{2}$	$1\ \bar{6}\ 3$ $\bar{3}\ \bar{3}\ \bar{9}$ $7\ 0\ 0$

(Mints, Belyaeva & Malkov, 1962). For Ni_3Nb, we obtained from electron microscopy measurements $a'=5{\cdot}106$, $b=4{\cdot}226$, $c=4{\cdot}517$ Å. The initial orientations of the frames $F0$, $F1$, $F2$ are chosen such that $\mathbf{e}_i \| \mathbf{a}_i^1 \| \mathbf{a}_i^{2,0}$ ($i=1,2,3$). The expressions in $F0$ of the transformations S_1 and $\mathsf{S}_{2,0}$ are:

$$[\mathsf{S}_1]_{F0}=\begin{pmatrix} a & 0 & 0\\ 0 & a & 0\\ 0 & 0 & a\end{pmatrix}\quad [\mathsf{S}_{2,0}]_{F0}=\begin{pmatrix} a' & 0 & 0\\ 0 & b & 0\\ 0 & 0 & c\end{pmatrix}.$$

On stereographic projections, the representative points of vectors $\mathbf{V}^1$ are inside the triangle $[100]_1$, $[1\bar{1}0]_1$, $[1\bar{1}1]_1$, while for $\mathbf{V}^2$ the representative points are inside the triangle $[100]_2$, $[010]_2$, $[001]_2$. Setting $\Sigma_{1\,\max}=21$, $S_{\max}=0{\cdot}102$, $\Delta L=0{\cdot}5$ Å, we find 14 different axes of rotation. With the additional set of calculation parameters $\Delta u=0{\cdot}4$ and $\Delta\theta=0{\cdot}003$ rad, the computer now finds 18 different pairs of cells $M1$ and $M2$ (see Table 1). The program written in Fortran IV needs an execution time of 75 s on a Cyber 74 computer. Some of these pairs are found simultaneously for the same rotation $\mathbf{R}$ (rows 1,2,4). For such cases the greatest values of Σ_1 and Σ_2 are denoted in columns 1 and 2 in parentheses. Columns 3 to 11 relate only to the values of Σ_1 and Σ_2 not enclosed in parentheses.

Columns 3 to 6 specify successively: (i) the components of the base vectors of the cells $M1$ and $M2$ referred respectively to the frames $F1$ and $F2$; (ii) the symmetry of the lattice built on $M1$, deduced from Niggli's scalar representation of $M1$ (see, for instance, Buerger, 1957). The abbreviations or P, mo P, tri, mean, respectively, orthorhombic primitive, monoclinic primitive, triclinic lattice; (iii) the corresponding principal strains ε_1, ε_2, ε_3.

Column 7 gives the components in $F0$ of the rotation vector $\mathbf{R}_d$ (r_1, r_2, r_3) as well as the rotation angle $|\mathbf{R}_d|$ for which $M2$ can be deduced from $M1$ by a pure deformation. In some cases, pairs of cells have identical cells $M1$ with cells $M2$ differing only slightly by one or two angles, *e.g.* the two pairs for which $\Sigma_1=20$ and $\Sigma_2=9$.

Columns 8 and 9 specify the rational transformation $[\mathsf{U}]_{F1}$.

Columns 10 and 11 specify the components of the base vectors of the DSC-1 and DSC-2 lattices, with reference to frames $F1$ and $F2$ respectively.

For instance, for the most commonly observed relative orientation of the two phases in our eutectic samples, the base vectors are (line 3, Table 1, $\Sigma_1=12$ and $\Sigma_2=6$):

– for the DSC-1 lattice: $\frac{a}{6}(112)$, $\frac{a}{3}(11\bar{1})$, $\frac{a}{2}(\bar{1}10)$

– for the DSC-2 lattice: $\frac{c}{3}(001)$, $\frac{b}{2}(010)$, $\frac{a'}{2}(\bar{1}00)$.

It is worth noting that only three different $\mathbf{R}$ axes are needed to determine all the different pairs of cells $M1$ and $M2$. These axes are: $[1\bar{1}0]_1\|[100]_2$, $[1\bar{1}1]_1\|[011]_2$, $[2\bar{1}0]_1\|[111]_2$.

6. Example 2: Zn/Zn (Table 2)

The parameters of the hexagonal primitive cell of pure Zn are: $a=b=2{\cdot}664$, $c=4{\cdot}9461$ Å, $\alpha=\beta=\pi/2$, $\gamma=2\pi/3$ [Ancker (1953), cited by Donnay & Ondick (1973)]. As in example 1, the initial orientations of frames $F0$, $F1$, $F2$ are such that $\mathbf{e}_i \| \mathbf{a}_i^1 \| \mathbf{a}_i^{2,0}$. The expressions in $F0$ of transformations S_1 and S_2 are:

$$[\mathsf{S}_1]_{F0}=[\mathsf{S}_{2,0}]_{F0}=\begin{pmatrix} a & -a/2 & 0\\ 0 & (a\sqrt{3})/2 & 0\\ 0 & 0 & c\end{pmatrix}.$$

Choosing $\Sigma_{1\,\max}=25$, $S_{\max}=0{\cdot}021$, $\Delta L=0{\cdot}5$ Å leads to 24 different axes $\mathbf{V}^1\|\mathbf{V}^2$. With the additional set of calculation parameters $\Delta u=0{\cdot}3$ and $\Delta\theta=0{\cdot}003$ rad, the computer finds 23 different pairs of cells $M1$ and $M2$ for which $\Sigma_1=\Sigma_2=N=\Sigma$ (see Table 2).

The results obtained by Bruggeman *et al.* (1971) for Zn are included in Table 2, as are those of Warrington (1975), which relate to the three solutions $\Sigma=7,13,19$, for which $\varepsilon_1=\varepsilon_2=\varepsilon_3=0$. Rotations $\mathbf{R}$ are found which may define, as above, more than one pair of cells $M1$ and $M2$ (rows 4,5,6,9). The columns 2 to 9 relate only to the values of Σ not enclosed in parentheses. The symmetry of the lattice built on $M1$ is denoted by one of the abbreviations hex, rh, mo P, mo C or tri which mean respectively hexagonal, rhombohedral, monoclinic primitive, side-centred monoclinic, triclinic.

For this second example six $\mathbf{R}$ axes are needed to determine the 24 pairs of cells $M1$ and $M2$. These axes are [100], [210], [001], [310], [201], [311].

Conclusion

A computer technique has been developed leading to the determination of all different pairs of non-primitive cells $M1$ and $M2$ of lattices 1 and 2 which can be approximately or exactly superposed for suitable relative orientations of the two lattices. For each pair of cells, the program determines an orientation of lattice 2 for which $M2$ can be deduced from $M1$ by a pure deformation. If lattices 1 and 2 are the same, the computing method gives all the twin orientations.

The program can treat two triclinic cells without difficulty. Applied to reciprocal lattices, the program can find directly the orientation relations giving rise to a high coincidence of dense direct lattice planes. Convenient base vectors for the DSC-1 and DSC-2 lattices are determined which are necessary to determine the Burgers vectors of intrinsic phase- (or grain-) boundary dislocations.

The method has been applied to the crystal lattices of Ni_3Al (cubic) and Ni_3Nb (orthorhombic) up to Σ (Ni_3Al)$=21$ and Σ (Ni_3Nb)$=10$, and to two lattices of Zn (hexagonal) up to Σ (Zn)$=25$. For these examples, the execution time of the program is about 75 s with a Cyber 74 computer.

The examples treated show that for certain orientation relations several different pairs of cells $M1$ and $M2$ with small values of Σ_1, Σ_2 (or $\Sigma_1 = \Sigma_2 = \Sigma$), may be in near coincidence simultaneously. In these cases, different DSC-1 and DSC-2 lattices may be calculated for the corresponding orientation relations.

Table 2. *Near (and exact) concident cells $M1$ and $M2$ for two lattices of* Zn *and related crystallographic quantities. Computation performed for $\Sigma_{1\,max} = 25$, $\Delta L = 0{\cdot}5$ Å, $S_{max} = 0{\cdot}021$, $\Delta u = 0{\cdot}3$, $\Delta\theta = 0{\cdot}003$ rad*

Σ	M1 $[U_1]_{F_1}$	M2 $[U_2]_{F_2}$	Sym M1	ε_1 ε_2 ε_3	R_d {r_1, r_2, r_3} (rd) $\lvert R_d \rvert$	$[U]_{F_1}$ ×Σ	$[DSC1]_{F_1}$ ×Σ	$[DSC2]_{F_2}$ ×Σ
7	0 $\bar{2}$ 1 0 1 3 $\bar{1}$ 0 0	0 $\bar{3}$ $\bar{1}$ 0 $\bar{1}$ 2 $\bar{1}$ 0 0	hex	0 0 0	0 0 -0.667 0.667	3 5 0 $\bar{5}$ 8 0 0 0 7	$\bar{2}$ 1 0 1 3 0 0 0 $\bar{7}$	$\bar{3}$ $\bar{1}$ 0 $\bar{1}$ 2 0 0 0 $\bar{7}$
9	$\bar{1}$ 1 1 0 3 3 0 1 $\bar{2}$	$\bar{1}$ 1 $\bar{2}$ 0 3 $\bar{3}$ 0 $\bar{1}$ $\bar{2}$	mo C	-0.010 0 0.010	1.231 0 0 1.231	9 $\bar{3}$ $\bar{9}$ 0 3 $\bar{18}$ 0 4 3	3 3 $\bar{6}$ 6 $\bar{3}$ $\bar{3}$ $\bar{1}$ $\bar{1}$ $\bar{1}$	0 3 $\bar{6}$ 0 $\bar{3}$ $\bar{3}$ $\bar{3}$ 1 1
9 (22)	2 0 1 1 $\bar{1}$ $\bar{3}$ 0 1 $\bar{1}$	2 0 1 1 1 $\bar{3}$ 0 1 1	mo C	-0.006 0 0.007	0.850 0.491 0 0.982	9 0 0 2 5 $\bar{14}$ $\bar{2}$ 4 5	0 0 9 $\bar{1}$ $\bar{7}$ 1 1 $\bar{2}$ $\bar{1}$	0 0 9 1 $\bar{7}$ 1 1 2 1
11 (17)	$\bar{1}$ 0 4 0 1 9 0 1 $\bar{2}$	$\bar{1}$ $\bar{1}$ 4 0 $\bar{1}$ 9 0 1 2	mo C	-0.008 0 0.008	-0.881 0 0 0.881	11 $\bar{2}$ 9 0 7 18 0 $\bar{4}$ 7	$\bar{1}$ 5 $\bar{5}$ $\bar{2}$ $\bar{1}$ $\bar{10}$ $\bar{2}$ $\bar{1}$ 1	1 6 $\bar{4}$ 2 1 $\bar{8}$ $\bar{2}$ $\bar{1}$ $\bar{3}$
13 (15)	1 $\bar{1}$ $\bar{3}$ 0 $\bar{2}$ $\bar{7}$ 0 1 $\bar{3}$	1 1 $\bar{3}$ 0 2 $\bar{7}$ 0 1 3	mo C	-0.008 0 0.008	1.494 0 0 1.494	13 $\bar{6}$ $\bar{14}$ 0 1 $\bar{28}$ 0 6 1	1 $\bar{3}$ 10 2 7 7 $\bar{1}$ 3 3	$\bar{1}$ $\bar{3}$ 10 $\bar{2}$ 7 7 $\bar{1}$ $\bar{3}$ $\bar{3}$
13	0 $\bar{1}$ $\bar{4}$ 0 3 $\bar{1}$ 1 0 0	0 $\bar{3}$ $\bar{4}$ 0 1 $\bar{3}$ 1 0 0	hex	0 0 0	0 0 -0.562 0.562	7 8 0 $\bar{8}$ 15 0 0 0 13	1 4 0 $\bar{3}$ 1 0 0 0 13	3 4 0 $\bar{1}$ 3 0 0 0 13
15	$\bar{2}$ $\bar{1}$ 0 $\bar{1}$ $\bar{1}$ $\bar{7}$ 0 $\bar{1}$ 1	$\bar{2}$ $\bar{1}$ 0 $\bar{1}$ 0 $\bar{7}$ 0 $\bar{1}$ $\bar{1}$	mo C	-0.004 0 0.004	-0.452 -0.261 0 0.522	15 0 0 1 13 14 2 $\bar{4}$ 13	0 0 $\bar{15}$ 1 7 $\bar{7}$ 2 $\bar{1}$ 1	0 0 $\bar{15}$ $\bar{1}$ 7 $\bar{8}$ 2 1 1
15 (23)	$\bar{2}$ $\bar{1}$ $\bar{1}$ $\bar{1}$ $\bar{2}$ 4 0 1 2	$\bar{2}$ $\bar{1}$ $\bar{1}$ $\bar{1}$ 1 4 0 1 $\bar{2}$	mo C	-0.010 0 0.010	1.186 0.685 0 1.369	15 0 0 6 3 $\bar{27}$ $\bar{4}$ 8 3	0 0 15 3 6 9 $\bar{2}$ 1 $\bar{1}$	0 0 15 $\bar{3}$ 3 6 $\bar{2}$ $\bar{3}$ $\bar{1}$
15	$\bar{2}$ 0 $\bar{1}$ $\bar{1}$ $\bar{2}$ $\bar{4}$ 0 $\bar{1}$ 2	$\bar{2}$ 0 $\bar{1}$ $\bar{1}$ $\bar{2}$ 3 0 1 2	mo C	-0.008 0 0.008	1.303 0.752 0 1.504	15 0 0 7 1 $\bar{28}$ $\bar{4}$ 8 1	0 0 $\bar{15}$ $\bar{2}$ $\bar{7}$ $\bar{11}$ $\bar{1}$ 4 2	0 0 $\bar{15}$ $\bar{2}$ 7 $\bar{4}$ 1 4 2
17	$\bar{1}$ 1 $\bar{5}$ $\bar{1}$ $\bar{1}$ 4 0 1 4	0 2 9 1 1 5 0 1 $\bar{4}$	mo C	-0.010 0 0.010	1.765 0 1.621 2.397	8 $\bar{17}$ 18 9 $\bar{17}$ $\bar{18}$ 8 0 1	$\bar{1}$ 13 $\bar{4}$ 1 4 $\bar{13}$ $\bar{1}$ $\bar{4}$ $\bar{4}$	$\bar{2}$ $\bar{9}$ $\bar{9}$ $\bar{1}$ $\bar{13}$ 4 $\bar{1}$ 4 4
18	$\bar{1}$ $\bar{2}$ $\bar{3}$ 0 $\bar{4}$ $\bar{6}$ 0 $\bar{1}$ 3	$\bar{1}$ $\bar{2}$ 1 0 $\bar{4}$ 2 0 1 4	mo P	-0.002 0 0.002	0.982 0 0 0.982	18 $\bar{4}$ $\bar{16}$ 0 $\bar{10}$ $\bar{32}$ 0 7 10	2 $\bar{12}$ 6 4 $\bar{6}$ $\bar{6}$ 1 3 3	2 $\bar{8}$ 10 4 2 2 $\bar{1}$ 4 4
19	$\bar{1}$ $\bar{1}$ $\bar{5}$ 0 $\bar{1}$ $\bar{9}$ 0 $\bar{2}$ 1	$\bar{1}$ 0 $\bar{5}$ 0 1 $\bar{9}$ 0 $\bar{2}$ $\bar{1}$	mo C	-0.005 0 0.005	-0.463 0 0 0.463	19 $\bar{1}$ 9 0 17 18 0 $\bar{4}$ 17	1 5 $\bar{9}$ 2 10 1 4 1 2	$\bar{1}$ 4 $\bar{10}$ $\bar{2}$ 8 $\bar{1}$ 4 3 2
19	0 $\bar{3}$ 2 0 2 5 $\bar{1}$ 0 0	0 $\bar{5}$ $\bar{2}$ 0 $\bar{2}$ 3 $\bar{1}$ 0 0	hex	0 0 0	0 0 -0.817 0.817	5 16 0 $\bar{16}$ 21 0 0 0 19	3 $\bar{2}$ 0 $\bar{2}$ $\bar{5}$ 0 0 0 $\bar{19}$	5 2 0 2 $\bar{3}$ 0 0 0 $\bar{19}$
21	2 1 1 1 $\bar{1}$ 5 0 $\bar{2}$ $\bar{1}$	2 1 1 1 2 5 0 $\bar{2}$ 1	mo C	-0.007 0 0.007	-0.671 -0.388 0 0.775	21 0 0 3 15 27 4 $\bar{8}$ 15	0 0 21 6 $\bar{3}$ 9 1 3 $\bar{2}$	0 0 21 3 $\bar{6}$ 12 3 1 $\bar{2}$
21	2 1 $\bar{3}$ 3 $\bar{2}$ $\bar{1}$ $\bar{1}$ $\bar{1}$ $\bar{1}$	1 $\bar{2}$ $\bar{3}$ $\bar{2}$ $\bar{3}$ $\bar{1}$ $\bar{1}$ 1 $\bar{1}$	rh	-0.007 0 0.007	1.212 0.420 0.907 1.571	22 $\bar{17}$ 14 19 $\bar{8}$ $\bar{28}$ 2 8 7	1 $\bar{9}$ $\bar{12}$ $\bar{2}$ $\bar{3}$ $\bar{18}$ 2 3 $\bar{3}$	2 $\bar{1}$ $\bar{18}$ 3 9 $\bar{6}$ 2 $\bar{1}$ 3
21	2 1 $\bar{3}$ 3 $\bar{2}$ $\bar{1}$ $\bar{1}$ $\bar{1}$ $\bar{1}$	$\bar{1}$ 2 $\bar{3}$ 2 3 $\bar{1}$ 1 $\bar{1}$ $\bar{1}$	rh	-0.007 0 0.007	-1.212 -0.420 -0.907 1.571	8 11 28 $\bar{9}$ 6 42 8 $\bar{10}$ 7	2 3 18 3 $\bar{6}$ 6 2 3 $\bar{3}$	1 10 12 $\bar{2}$ 1 18 2 $\bar{1}$ 3
23	$\bar{1}$ $\bar{1}$ $\bar{4}$ 0 $\bar{2}$ $\bar{7}$ 0 $\bar{3}$ 1	$\bar{1}$ 1 $\bar{4}$ 0 2 $\bar{7}$ 0 $\bar{3}$ $\bar{1}$	mo C	-0.004 0 0.004	-0.599 0 0 0.599	23 $\bar{2}$ 14 0 19 28 0 $\bar{6}$ 19	$\bar{1}$ $\bar{7}$ $\bar{15}$ $\bar{2}$ $\bar{14}$ $\bar{7}$ $\bar{3}$ 2 1	1 $\bar{7}$ $\bar{15}$ 2 $\bar{14}$ $\bar{7}$ $\bar{3}$ $\bar{2}$ $\bar{1}$
25	$\bar{2}$ 0 $\bar{1}$ $\bar{1}$ $\bar{3}$ $\bar{4}$ 0 $\bar{1}$ 3	$\bar{2}$ 0 $\bar{1}$ $\bar{1}$ $\bar{3}$ 3 0 1 3	mo C	-0.007 0 0.007	0.966 0.558 0 1.115	25 0 0 7 11 $\bar{42}$ $\bar{6}$ 12 11	0 0 $\bar{25}$ $\bar{3}$ $\bar{7}$ $\bar{16}$ $\bar{1}$ 6 3	0 0 $\bar{25}$ $\bar{3}$ 7 $\bar{9}$ 1 6 3
25	3 0 2 1 $\bar{3}$ 3 0 $\bar{1}$ $\bar{2}$	3 0 1 1 $\bar{3}$ $\bar{2}$ 0 1 $\bar{2}$	tri	-0.009 0 0.009	1.054 0.365 0.0 1.115	26 $\bar{3}$ $\bar{9}$ 5 10 $\bar{45}$ $\bar{4}$ 12 11	$\bar{6}$ $\bar{1}$ $\bar{7}$ $\bar{5}$ $\bar{5}$ 15 $\bar{1}$ 4 3	$\bar{6}$ 1 $\bar{8}$ $\bar{5}$ 5 10 1 4 $\bar{7}$

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APPENDIX

Let us consider a multiple cell M of a lattice Λ, M being a Niggli reduced cell. If the six parameters of M are a, b, c, α, β, γ with $|\mathbf{a}| \le |\mathbf{b}| \le |\mathbf{c}|$ the volume of M is

$$V = abc(1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma)^{1/2}. \quad (1a)$$

From this equation and the property that the three angles α, β, γ cannot deviate from $\pi/2$ by more than 30° (Balashov & Ursell, 1957), we derive the inequality:

$$V \ge a^3/(2)^{1/2}. \quad (2a)$$

Denoting by Σ the ratio V/v, where v is the volume of a primitive cell of lattice Λ, we deduce the following inequality:

$$a \le (\Sigma\, v)^{1/3} 2^{1/6}. \quad (3a)$$

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On the Conditional Probability of Quintets

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A new expression for the conditional probability distribution of quintet structure invariants is given, which in exponential approximation reduces to the exponential expression of Hauptman & Fortier [*Acta Cryst.* (1977), A**33**, 575–580]. In a practical example the expression gave promising results.

Introduction

Several expressions for the conditional probability distributions (c.p.d.) of quartet and quintet structure invariants have been reported, some of which have a purely exponential form while others contain Bessel functions as well.

For quartets the theory is well established. For the magnitudes of the reflexions H, K, L, $H+K+L$, $H+K$, $H+L$, $K+L$ Hauptman (1975) derived the expression

$$P(|\varphi_4|)=L\exp(-4E_4\cos\varphi_4)I_0(2N^{-1/2}|E_{H+K}|Z_{HK})\times I_0(2N^{-1/2}|E_{H+L}|Z_{HL})I_0(2N^{-1/2}|E_{K+L}|Z_{KL}) \quad (1)$$

in which L is a suitable normalizing constant,

$$E_4=N^{-1}|E_HE_KE_LE_{H+K+L}|,$$
$$\varphi_4=\varphi_H+\varphi_K+\varphi_L+\varphi_{-H-K-L},$$

I_0 is a modified Bessel function and

$$Z_{HK}=(E_H^2E_K^2+E_L^2E_{H+K+L}^2+2NE_4\cos\varphi_4)^{1/2}.$$

Dependent on the seven $|E|$ values a maximum value of $P(|\varphi_4|)$ corresponds to a phase $|\varphi_4|$ anywhere in the range $0\le|\varphi_4|\le\pi$.

A second expression for the c.p.d. of quartets is derived by Giacovazzo (1976):

$$P(|\varphi_4|)=L'\exp[-2E_4(2-E_{H+K}^2-E_{H+L}^2-E_{K+L}^2)\cos\varphi_4] \quad (2)$$

in which L' is a suitable normalizing constant. This formula has maxima for $\varphi_4=0$ or π only.

Making use of

$$I_0(z)\simeq\exp\left(\frac{z^2}{4}\right), \quad (3)$$

which is valid for small values of z, Heinerman (1976) (see also Giacovazzo, 1977) has shown that (2) is an approximation of (1). Test results (Schenk, 1977) show that (1) leads to phase estimates with smaller errors than (2) does.

For the estimation of phases

$$|\varphi_5|=|\varphi_H+\varphi_K+\varphi_L+\varphi_M+\varphi_{-H-K-L-M}|$$

of quintet relations several procedures and expressions have been described (Schenk, 1975; Schenk & van der Putten, 1976; Krabbendam, 1976; van der Putten & Schenk, 1976; Hauptman & Fortier, 1977).

Among the purely exponential expressions the one of Hauptman & Fortier (1977) looks the most promising.

$$P(|\varphi_5|)=C\exp[(\sum_{15\text{ terms}}E_{H+K}^2E_{L+M}^2-2\sum_{10\text{ terms}}E_{H+K}^2+6)2E_5\cos\varphi_5]. \quad (4)$$

Here C is a suitable normalizing constant, the sums are taken over all combinations of the 10 cross-reflexions $H+K$ *etc.* and

$$E_5=N^{-3/2}|E_HE_KE_LE_ME_{H+K+L+M}|.$$

Like its quartet analogue (2) this formula gives values for $|\varphi_5|$ of 0 and π only.

The mixed exponential–Bessel formulae for quintets reported so far are proposed on the basis of the purely exponential expressions. It was stated by Hauptman & Fortier (1977) that: 'it is therefore plausible to as-