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Coincidence-Site Lattices and Complete Pattern-Shift Lattices in Cubic Crystals

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Two interpenetrating point lattices contain under certain conditions a common sublattice, *i.e.* a 'coincidence-site lattice' (CSL). The present study is restricted to cubic lattices [primitive cubic (p.c.), f.c.c. and b.c.c.]. It is shown that it is necessary for the existence of a CSL that the two lattices are related by a rotation **R** represented by a rational matrix in the cubic coordinate system of one of the lattices. It is further shown that the common denominator N in **R** is equal to the ratio Σ of the unit volume of the CSL referred to the unit volume of the crystal lattice. The 'complete pattern-shift lattice' (DSCL) is defined as the coarsest lattice which, in CSL orientation, contains both crystal lattices as sublattices. Further it is proved that the volume of the DSCL unit referred to the crystal unit is $1/\Sigma$ and that for the p.c. structure the CSL and the DSCL are reciprocal lattices. For both f.c.c. and b.c.c. the CSL and the DSCL have to be face-centred or body-centred respectively. Methods are described for all three cases to determine explicitly the CSL, the DSCL and the planar density of coincidence sites. A table is given for **R**, the CSL's and the DSCL's up to $\Sigma = 49$. This study is of importance for the investigation of grain boundaries in cubic crystals.

Introduction

Coincidence-site lattices are of importance in connexion with the study of grain boundaries. Although grain boundaries are two-dimensional features it is useful to investigate three-dimensional configurations of the interpenetrating point lattices numbers 1 and 2 and later interpret the grain boundary as a two-dimensional section through this configuration. For convenience we place the lattices so that they have at least one point in common, which is called a coincidence site, and choose that point as origin. If there exist more coincidence sites, then owing to the periodicity of the two crystal lattices, there exists a whole coincidence-site lattice, (CS lattice or CSL). The CSL is the finest common sublattice of the crystal lattices 1 and 2.

The existence of a CSL indicates that the pattern formed by the lattice points of both crystal lattices is periodic with the periodicity of the CSL. Other periodic patterns with the same period but without containing a CSL can be produced by translation of lattice 2 with respect to crystal 1 (Bollmann, 1970).

For the structure of grain boundaries it is of importance that, of all the patterns obtained by translation, one has the lowest energy, and that crystals tend to conserve that pattern, which may or may not be the one with the CSL. Hence, when talking of CSL's we have to understand these primarily as periods of patterns, and the CSL's are convenient representations of these periods.

In addition to the CSL we shall consider the coarsest lattice that contains crystal lattice 1 and 2 as sublattices. This is called the 'complete pattern-shift lattice' or DSC lattice [*D* stands for *d*isplacement of lattice 2 (lattice 1 is always considered as fixed), *S* for *s*hift of the pattern and *C* for *c*omplete]. The DSC lattice is composed of all the translations of lattice 2 that leave the structure of the (periodic) pattern unchanged.

A slight deviation in the relative orientation of the two crystals away from a coincidence orientation produces a network of so called 'secondary dislocations', which allow the crystal to conserve the minimum-energy pattern over most of the boundary surface. The existence of such networks was shown among others by Schober & Balluffi (1970, 1971) and Bollmann, Michaut & Sainfort (1972). Warrington & Bollmann (1972) have shown that secondary dislocation networks can be calculated by exactly the same procedure as low-angle boundaries, except that the crystal lattices have to be replaced by DSC lattices and that the angular deviation of the crystal lattices has to be replaced by the deviation from the coincidence orientation. The shortest translation vectors of the DSC lattice are the Burgers vectors of the secondary dislocations.

In this paper, we shall consider only the case that lattice 1 has cubic symmetry. The reason is that for cubic symmetry there are a particularly large number of rotations that lead to a large density of coincidence sites.

In general, it is expected that a high-angle interface is favoured energetically if the coincidence sites are dense in the plane of the interface. One reason for us to look at the arrangement of coincidence points in three-dimensional space and not just in a given plane is that the spatial arrangement for a given rotation allows us to recognize at once all the planes with a high density of coincidence sites. This is important because the interface between two grains may not be

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planar. In the case of a cubic lattice 1, the coincidence sites form a three-dimensional lattice if they do not all lie on a straight line. Moreover, the area A of a primitive cell of the sublattice of the CSL in a given plane can be small only if the volume V of a primitive cell of the whole CSL is small too. [It can be shown that $aV \leq A^2$ for a primitive cubic (p.c.) lattice with lattice constant a.]

We give here a few indications on the historical development of the coincidence concept in connexion with grain boundaries. The coincidence concept was apparently first noted by Friedel (1964) with respect to twin orientations. A number of theoretical investigations of the properties of coincidence-site lattices were subsequently made (Brandon, Ralph, Ranganathan & Wald, 1964; Ranganathan, 1966; Brandon, 1966; Bishop & Chalmers, 1968; Tu, 1971; Pumphrey & Bowkett, 1971; Fortes, 1972; Woirgard & de Fouquet, 1972; Santoro & Mighell, 1973). Experimental evidence that a grain boundary in coincidence orientation can be a local minimum of energy has been given by Schober & Balluffi (1970, 1971) and by Chaudhari & Matthews (1970, 1971).

We divide our paper into two parts. Part I uses elementary number-theoretical methods, which are convenient for deriving general results about the CS and DSC lattices. They also permit the explicit calculation of these lattices.

Part II describes the procedure for calculating the CSL and the DSCL based on the 0-lattice theory by methods of matrix calculation for the p.c., f.c.c. and b.c.c. lattices. It also shows the method for calculating the density of coincidence sites on a given plane. At the end is given a table which contains the CSL's and DSCL's for values of Σ up to 49.

PART I

1.1 The rotation matrix

We choose a coordinate system with axes parallel to the edges of a standard cubic unit cell of lattice 1 and we choose the length of an edge as length unit. Following Warrington & Bufalini (1971) we consider rotations that, in our coordinate system, are described by a matrix **R** with rational matrix elements. We can write

$$\mathbf{R}=\frac{1}{N}\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \qquad (1\text{-}1)$$

such that there is no integral factor common to the positive integer N and the nine integers a_{ij}. Since **R** is an orthogonal matrix, we have

$$\sum_{k=1}^{3} a_{ik}a_{jk}=N^2\delta_{ij} \quad \text{and} \quad \sum_{k=1}^{3} a_{ki}a_{km}=N^2\delta_{im}\,, \qquad (1\text{-}2)$$

where $\delta_{ij}=1$ if $i=j$, $\delta_{ij}=0$ otherwise. The equations (1-2) imply $a_{i1}^2+a_{i2}^2+a_{i3}^2=N^2$ for $i=1$, 2 and 3. $a_{i1}^2+a_{i2}^2+a_{i3}^2$ is a number of the form $4n+k_i$, where n is an integer and k_i the number of odd integers among a_{i1}, a_{i2}, a_{i3}, *i.e.* $k_i=0$, 1, 2, or 3. If N is even, then N^2 is a multiple of 4 and $N^2=4n+k_i$ implies $k_i=0$ for $i=$ 1, 2, and 3. However, according to our convention, N and the nine numbers a_{ij} cannot all be even. We conclude that N is odd.

The angle θ of the rotation described by the matrix **R** is determined by the trace t of **R**

$$t=N^{-1}(a_{11}+a_{22}+a_{33})=2\cos\theta+1\,. \qquad (1\text{-}3)$$

The rotation axis points in the direction of the vector $\mathbf{c}=\{a_{32}-a_{23}, a_{13}-a_{31}, a_{21}-a_{12}\}$. The angle of rotation lies between 0 and 180° and forms a right-hand screw with respect to **c**.

1.2 Notation and summary of part I

We shall use Λ to refer to a lattice. The superscripts p, f and b distinguish between primitive cubic (p.c.), face-centred cubic (f.c.c.), and body-centred cubic (b.c.c.) lattices; the subscripts 1, 2, C and D distinguish between lattice 1, lattice 2, the CSL, and the DSCL. By V we denote the volume of a primitive cell of Λ. Notice that we have chosen a coordinate system such that $V_1^p=1$, $V_1^f=\frac{1}{4}$, $V_1^b=\frac{1}{2}$. By G we denote the group of translation vectors that leave the lattice Λ invariant: by a basis for G we understand a set of three translation vectors $\mathbf{e}_1$, $\mathbf{e}_2$, and $\mathbf{e}_3$ such that each vector in G can be written as a linear combination with integral coefficients of $\mathbf{e}_1$, $\mathbf{e}_2$, and $\mathbf{e}_3$. The matrix of which the ith column gives the components of $\mathbf{e}_i$ will be called a basis matrix and denoted by $[\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3]$.

A central role in our paper is played by the following theorem, where N is the denominator introduced in the expression (1-1) for **R**.

Theorem 1

$$V_C^p=NV_1^p\,. \qquad (1\text{-}4)$$

The ratio V_C/V_1 is usually called Σ in the literature. The proof that $\Sigma=N$ if lattice 1 is p.c. is given in the Appendix because it requires mathematical tools that will not be familiar to every reader. We have written the Appendix sufficiently self-contained for it to be read before § 1.3 and the following sections, where Theorem 1 will be taken for granted. In § 1.3 we shall show that $V_C=NV_1$ also if lattice 1 is f.c.c. or b.c.c., *i.e.* $\Sigma=N$ for all three types of cubic lattice. § 1.4 contains the proof that $V_D=N^{-1}V_1$ in all three cases and that Λ_C^p and Λ_D^p are reciprocal lattices. In § 1.5 we shall determine Λ_C^p explicitly by giving a basis for this lattice. Once a basis for Λ_C^p is known, it is easy to find bases for the other CSL and for the DSC lattices. The procedures are described in §§ 1.3 and 1.4 as indicated in Fig. 1.

1.3 The coincidence-site lattice Λ_C

$\mathbf{v} \in G_C$ (*i.e.* **v** is a vector in the group G_C) if and only if $\mathbf{v} \in G_1$ and $\mathbf{v} \in G_2$. The condition $\mathbf{v} \in G_2$ is equivalent

to $\mathbf{R}^{-1}\mathbf{v} \in G_1$. Therefore we obtain the result

$$\mathbf{v} \in G_C \quad \text{if and only if} \quad \mathbf{v} \in G_1 \quad \text{and} \quad \mathbf{R}^{-1}\mathbf{v} \in G_1 ,$$

which will repeatedly be used in the sequel.

1.3.1 *Properties of Λ_C^p*

In this subsection we shall discuss properties of Λ_C^p that we shall need to compare Λ_C^p with Λ_C^f and Λ_C^b.

G_C^p contains vectors with all three components even, *e.g.*, $\{0,0,0\}$. They form a subgroup H of G_C^p. If G_C^p contains vectors of type $\{d,e,e\}$, *i.e.* with the first component od*d* and the other two components *e*ven, then these vectors form a coset of the subgroup H of G_C^p. [This can be seen as follows: let $\mathbf{u},\mathbf{v} \in G_C^p$, $\mathbf{u}$ of type $\{d,e,e\}$ then $\mathbf{u}-\mathbf{v} \in H$ if and only if $\mathbf{v}$ is of type $\{d,e,e\}$.] In this way one finds that there can be at most eight cosets of the subgroup H of G_C^p, which correspond to the vectors of type

$$\begin{pmatrix} e \\ e \\ e \end{pmatrix} \quad \begin{pmatrix} d \\ e \\ e \end{pmatrix} \quad \begin{pmatrix} e \\ d \\ e \end{pmatrix} \quad \begin{pmatrix} e \\ e \\ d \end{pmatrix} \quad \begin{pmatrix} e \\ d \\ d \end{pmatrix} \quad \begin{pmatrix} d \\ e \\ d \end{pmatrix} \quad \begin{pmatrix} d \\ d \\ e \end{pmatrix} \quad \begin{pmatrix} d \\ d \\ d \end{pmatrix} . \tag{1-5}$$

The number of cosets of the subgroup H of G equals the number of elements in the factor group G/H, called ord (G/H). These group-theoretical notions have the following interpretation in terms of lattices. Let Λ be the lattice connected with G. Each coset corresponds to a sublattice of Λ with H as the group of its translation vectors. The sublattices of Λ connected with two different cosets are related by a translation; ord (G/H) equals the number of superimposed sublattices that make up Λ.

We have proved ord $(G_C^p/H) \leq 8$. Next we shall show ord $(G_C^p/H) \geq 8$, so that we can conclude that G_C^p in fact contains elements of all the eight types distinguished in (1-5). The volume of a primitive cell of the lattice determined by H is a multiple of 8 whereas V_C^p is an odd integer because $V_C^p = N$ by Theorem 1. It follows that ord (G_C^p/H) is a multiple of eight.

Consider a basis $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ of G_C^p. Every vector in G_C^p has the form $\lambda_1\mathbf{e}_1 + \lambda_2\mathbf{e}_2 + \lambda_3\mathbf{e}_3$, where the λ_is are integers. $\lambda_1\mathbf{e}_1 + \lambda_2\mathbf{e}_2 + \lambda_3\mathbf{e}_3$ and $\mu_1\mathbf{e}_1 + \mu_2\mathbf{e}_2 + \mu_3\mathbf{e}_3$ are of the same type if $\lambda_i - \mu_i$ is even for $i = 1$, 2, and 3. Therefore, the eight vectors we obtain if we let each of the coefficients λ_i take the values 0 or 1, contain representatives of every type of vector that appears in G_C^p. Since G_C^p contains vectors of all the eight types enumerated in (1-5), the eight vectors constructed must all have different types. The determinant of the basis matrix $[\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3]$ determines V_C^p, $\det [\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3] = \pm N$. Three vectors $\mathbf{f}_1$, $\mathbf{f}_2$, and $\mathbf{f}_3$ in G_C^p form a basis of G_C^p if and only if there exists a 3×3 matrix $\mathbf{U}$ with integral elements and determinant ± 1 such that $[\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3] = [\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3] \cdot \mathbf{U}$.

Vectors with integral components will be called of class k with k being the number of the odd components. We have to distinguish four classes:

The class	contains the type
0	$\{e,e,e\}$
1	$\{d,e,e\}$, $\{e,d,e\}$, $\{e,e,d\}$
2	$\{e,d,d\}$, $\{d,e,d\}$, $\{d,d,e\}$
3	$\{d,d,d\}$.

$v_1^2 + v_2^2 + v_3^2$, the square of the length of a vector $\mathbf{v}$ of class k has the form $4n + k$, n an integer. Since a rotation leaves the length unchanged, we conclude that for a vector $\mathbf{v} \in G_C^p$, $\mathbf{v}$ and $\mathbf{R}^{-1}\mathbf{v}$ belong to the same class.

1.3.2 *How big are V_C^f and V_C^b?*

G_1^b, the group that corresponds to a b.c.c. lattice 1, consists of G_1^p and of the vectors $\mathbf{u}$ with the property that $2\mathbf{u}$ is a vector in G_1^p of class 3. The length squared of $\mathbf{u}$ has the form $n + \frac{3}{4}$, n an integer, whereas the square of the length of a vector in G_1^p is integral. G_1^f consists of G_1^p and of the vectors $\mathbf{v}$ such that $2\mathbf{v}$ is a vector in G_1^p of class 2. The length squared of $\mathbf{v}$ is $n + \frac{1}{2}$.

Only f.c.c. lattices will be discussed in detail because b.c.c. lattices can be treated similarly. Choose in G_C^p a vector of type $\{e,d,d\}$, one of type $\{d,e,d\}$, and one of type $\{d,d,e\}$ and call them $\mathbf{u}_1$, $\mathbf{u}_2$, and $\mathbf{u}_3$ respectively. Let us write $\mathbf{u}_0$ for the vector $\{0,0,0\}$. The vectors $\frac{1}{2}\mathbf{u}_i$, $i = 0,1,2,3$ lie in G_C^f. Since G_C^f is a group, it follows that every vector $\mathbf{v}$ of the form $\mathbf{v} = \frac{1}{2}\mathbf{u}_i + \mathbf{a}$, where $i = 0$, 1, 2 or 3 and $\mathbf{a} \in G_C^p$, lies in G_C^f. We want to show that the converse is true, too. Take $\mathbf{b} \in G_C^f$. $\mathbf{b} - \frac{1}{2}\mathbf{u}_i \in G_C^f$ for $i = 0,1,2,3$. We can choose i such that the vector $\mathbf{c} = \mathbf{b} - \frac{1}{2}\mathbf{u}_i$ lies in G_1^p. $\mathbf{R}^{-1}\mathbf{c}$ lies in G_1^f and has the same length as $\mathbf{c}$. It follows that $\mathbf{R}^{-1}\mathbf{c} \in G_1^p$, *i.e.* $\mathbf{c} \in G_C^p$. This finishes the proof that $\mathbf{b} \in G_C^f$ has the form $\mathbf{b} = \frac{1}{2}\mathbf{u}_i + \mathbf{c}$, where $i = 0$, 1, 2, or 3 and $\mathbf{c} \in G_C^p$. There are four cosets of the subgroup G_C^p of G_C^f, each containing one of the vectors $\mathbf{u}_i$. Therefore, $V_C^f = \frac{1}{4}V_C^p = \frac{1}{4}NV_1^p = NV_1^f$.

Similarly one finds $V_C^b = \frac{1}{2}V_C^p = NV_1^b$. We conclude that Σ, the ratio V_C/V_1, satisfies $\Sigma = N$ for all the three kinds of cubic lattice.

1.3.3 *Explicit determination of Λ_C^f and Λ_C^b*

In § 1.5 it will be shown how to determine explicitly a basis $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ for G_C^p. Here we show how to change from a basis for G_C^p to bases for G_C^b or G_C^f.

b.c.c. One of the eight vectors $\lambda_1\mathbf{e}_1 + \lambda_2\mathbf{e}_2 + \lambda_3\mathbf{e}_3$, $\lambda_i = 0$ or 1, is of type $\{d,d,d\}$. We call this vector $\mathbf{u}$. Since only the vector of type $\{e,e,e\}$ has all three λ_i's equals to zero, it is possible to reorder the basis vectors, $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3 \rightarrow \mathbf{e}_1', \mathbf{e}_2', \mathbf{e}_3'$ such that $\lambda_1 = 1$. $\mathbf{u}, \mathbf{e}_2', \mathbf{e}_3'$ form a new basis of G_C^p. $\frac{1}{2}\mathbf{u}, \mathbf{e}_2', \mathbf{e}_3'$ are vectors in G_C^b; they form a basis of G_C^b because $\det [\frac{1}{2}\mathbf{u}, \mathbf{e}_2', \mathbf{e}_3'] = \frac{1}{2} \det [\mathbf{u}, \mathbf{e}_2', \mathbf{e}_3'] = \pm\frac{1}{2}N$.

f.c.c. Reorder the basis vectors, $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3 \rightarrow \mathbf{e}_1', \mathbf{e}_2', \mathbf{e}_3'$, so that the vector $\mathbf{v}$ of type $\{e,d,d\}$ has $\lambda_1 = 1$. $\{\mathbf{v}, \mathbf{e}_2', \mathbf{e}_3'\}$ form a basis for G_C^p. Interchange $\mathbf{e}_2'$ and $\mathbf{e}_3'$, $\mathbf{v}, \mathbf{e}_2', \mathbf{e}_3 \rightarrow \mathbf{v}, \mathbf{e}_2'', \mathbf{e}_3''$, if this is necessary in order that the vector $\mathbf{w}$ of type $\{d,e,d\}$ has $\lambda_2 = 1$. $\mathbf{v}, \mathbf{w}, \mathbf{e}_3''$ form a basis of G_C^p;

$\frac{1}{2}\mathbf{v}, \frac{1}{2}\mathbf{w}, \mathbf{e}_3''$ are vectors in G_C^f; they form a basis of G_C^f because $\det[\frac{1}{2}\mathbf{v}, \frac{1}{2}\mathbf{w}, \mathbf{e}_3''] = \pm\frac{1}{4}N$.

1.4 The complete pattern-shift lattice Λ_D

1.4.1 *The volume V_D of a primitive cell of Λ_D*

In this subsection we shall work with a crystal coordinate system of lattice 1; *i.e.* the coordinate system we use will depend on whether lattice 1 is p.c., f.c.c. or b.c.c. We shall determine V_D simultaneously for all the three cases. We write the components $\{a_1, a_2, a_3\}$ of a vector $\mathbf{a} \in G_2$ as $a_i = n_i + \alpha_i$, where n_i is an integer and $0 \leq \alpha_i < 1$ $(i = 1,2,3)$. $\{\alpha_1, \alpha_2, \alpha_3\}$ are called the reduced components of $\mathbf{a}$. $V_C = NV_1$ tells us that there are N cosets of the subgroup G_C of G_2. Vectors in the same coset have the same reduced components; vectors in different cosets have different reduced components. Hence, there are N different triples of reduced components. The group G_D consists of all vectors that have reduced components equal to one of the N triples. We conclude that $V_D = N^{-1}V_1$ in all three cases.

1.4.2 *Proof that Λ_C^p and Λ_D^p are reciprocal lattices*

Let $\mathbf{e}_1$, $\mathbf{e}_2$ and $\mathbf{e}_3$ be a basis for G_C^p.

$$\mathbf{e}_1^* = \frac{\mathbf{e}_2 \times \mathbf{e}_3}{N}, \quad \mathbf{e}_2^* = \frac{\mathbf{e}_3 \times \mathbf{e}_1}{N}, \quad \mathbf{e}_3^* = \frac{\mathbf{e}_1 \times \mathbf{e}_2}{N} \tag{1-6}$$

form a basis of the group G_R that corresponds to the reciprocal lattice Λ_R of Λ_C^p. Let $\mathscr{Z}$ denote the set of all integers. We want to show that G_R consists of all vectors $\mathbf{f}$ such that the scalar product $\mathbf{f} \,.\, \mathbf{v} \in \mathscr{Z}$ for all $\mathbf{v} \in G_C^p$. We do this by proving the following equivalent statement: G_R consists of all vectors $\mathbf{f}$ with $\mathbf{f} \,.\, \mathbf{e}_i \in \mathscr{Z}$ for $i = 1,2,3$. That $\mathbf{f} \,.\, \mathbf{e}_i \in \mathscr{Z}$ if $\mathbf{f} \in G_R$ is clear because

$$\mathbf{e}_i \,.\, \mathbf{e}_j^* = \delta_{ij} \,. \tag{1-7}$$

It remains to show that $\mathbf{f} \in G_R$ if $\mathbf{f} \,.\, \mathbf{e}_i \in \mathscr{Z}$ for $i = 1,2,3$. But this is true because for any vector $\mathbf{f}$:

$$\mathbf{f} = (\mathbf{f} \,.\, \mathbf{e}_1)\mathbf{e}_1^* + (\mathbf{f} \,.\, \mathbf{e}_2)\mathbf{e}_2^* + (\mathbf{f} \,.\, \mathbf{e}_3)\mathbf{e}_3^* \,. \tag{1-8}$$

In order to prove that G_D^p is contained in G_R we only have to show that $\mathbf{u} \,.\, \mathbf{v} \in \mathscr{Z}$ if $\mathbf{u} \in G_C^p$ and $\mathbf{v} \in G_D^p$. We can write $\mathbf{v} = \mathbf{v}_1 + \mathbf{v}_2$, where $\mathbf{v}_i \in G_i^p$, $i = 1,2$. $\mathbf{u} \,.\, \mathbf{v} = \mathbf{u} \,.\, \mathbf{v}_1 + \mathbf{u} \,.\, \mathbf{v}_2$. To complete the proof we notice $\mathbf{u} \,.\, \mathbf{v}_1 \in \mathscr{Z}$ because $\mathbf{u}, \mathbf{v}_1 \in G_1^p$ and $\mathbf{u} \,.\, \mathbf{v}_2 \in \mathscr{Z}$ because $\mathbf{u}, \mathbf{v}_2 \in G_2^p$. Since $V_C^p \,.\, V_R = 1$, we have $V_R = V_D^p$, so G_D^p must coincide with G_R, which proves that Λ_C^p and Λ_D^p are reciprocal lattices.

Notice that the relations (1.6) allow us to determine a basis for Λ_D^p once we know a basis $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ for Λ_C^p: if $\mathbf{M} := [\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3]$ then $[\mathbf{e}_1^*, \mathbf{e}_2^*, \mathbf{e}_3^*] = (\mathbf{M}^{-1})^T := \mathbf{M}^*$ (':=' stands for 'is by definition equal to'). $\mathbf{M}^*$ has the form $N^{-1}\mathbf{B}$, where $\mathbf{B}$ is a matrix with integral elements. Since $\det \mathbf{M}^* = \pm N^{-1}$ we have $\det \mathbf{B} = \pm N^2$.

1.4.3 *The lattices Λ_D^f and Λ_D^b*

Let G be the smallest group that contains $\mathbf{u}_1 := \{0, \frac{1}{2}, \frac{1}{2}\}$, $\mathbf{u}_2 := \{\frac{1}{2}, 0, \frac{1}{2}\}$, $\mathbf{u}_3 := \{\frac{1}{2}, \frac{1}{2}, 0\}$, and G_D^p. Obviously, G is contained in G_D^f. There are four cosets of the subgroup G_D^p of G, each containing one of the vectors $\mathbf{u}_i$, $i = 0,1,2,3$, where $\mathbf{u}_0 = \{0,0,0\}$. Since G and G_D both determine lattices the volume of a primitive cell of which is $\frac{1}{4} \,.\, V_D^p$, it follows that $G = G_D^p$.

Similarly one shows that G_D^b is the smallest group containing $\mathbf{u} := \{\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\}$ and G_D^p.

If $\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3$ form a basis for G_D^p then $N\mathbf{f}_1, N\mathbf{f}_2, N\mathbf{f}_3$ are vectors with integral components that span a volume N^2. Since N^2 is odd we can conclude, similarly as in § 1.3.1, that all the eight types (1-5) are represented among the eight vectors $N(\lambda_1\mathbf{f}_1 + \lambda_2\mathbf{f}_2 + \lambda_3\mathbf{f}_3)$, $\lambda_i = 0$ or 1. The procedure described in § 1.3.3 allows us to go over from the basis $\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3$

(1) to a basis $\mathbf{u}, \mathbf{f}_2', \mathbf{f}_3'$ such that $N\mathbf{u}$ has type $\{d,d,d\}$. $\frac{1}{2}\mathbf{u}, \mathbf{f}_2', \mathbf{f}_3'$ is a basis for G_D^b;

(2) to a basis $\mathbf{v}$, $\mathbf{w}$, $\mathbf{f}_3''$ such that $N\mathbf{v}$ has type $\{e,d,d\}$ and $N\mathbf{w}$ type $\{d,e,d\}$. $\frac{1}{2}\mathbf{v}, \frac{1}{2}\mathbf{w}, \mathbf{f}_3''$ is a basis for G_D^f.

1.5 An algorithm to determine Λ_C^p

We denote the largest common (integral) divisor of integers $a_1, \ldots, a_n$ by $(a_1, \ldots, a_n)$. Define $\alpha_1 := (a_{11}, a_{12}, N)$, $\alpha_2 := (a_{21}, a_{22}, N)$, where the a_{ij} are the matrix elements of $N \,.\, \mathbf{R}$. Lemma 2 in the Appendix states that $(\alpha_1, \alpha_2) = 1$. Let m_1 be the largest (integral) factor of N such that $(m_1, \alpha_1) = 1$. Define $m_2 = N/m_1$. It follows that $(m_1, m_2) = (m_2, \alpha_2) = 1$. Define $\delta_1 := (m_1, a_{11})$ and $\delta_2 := (m_2, a_{21})$. Notice that $(\delta_1, a_{12}) = (\delta_2, a_{22}) = 1$.

Let $a \underset{n}{\equiv} b$ state that $a - b$ is an (integral) multiple of n. In the Appendix we prove the following result: if $\mathbf{v}$ is a vector with integral components then $\mathbf{Rv}$ lies in G_C^p if and only if

$$\begin{aligned} &v_1a_{11} + v_2a_{12} + v_3a_{13} \underset{m_1}{\equiv} 0 \\ \text{and} \qquad &\\ &v_1a_{21} + v_2a_{22} + v_3a_{23} \underset{m_2}{\equiv} 0 \,. \end{aligned} \tag{1-9}$$

This result allows us to determine explicitly a basis $\mathbf{Rx}, \mathbf{Ry}, \mathbf{Rz}$ of G_C^p such that $\mathbf{x}, \mathbf{y}, \mathbf{z}$ has the form

$$\begin{pmatrix} x_1 & y_1 & z_1 \\ 0 & y_2 & z_2 \\ 0 & 0 & 1 \end{pmatrix}.$$

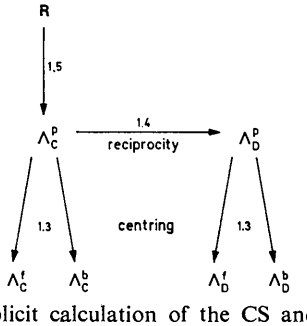

Fig. 1. The explicit calculation of the CS and DSC lattices. (The numbers refer to the sections of Part I where the procedure is described.)

First we shall describe an algorithm that yields values for x_1, y_1, y_2, z_1, z_2 and afterwards we shall show that the vectors **x**, **y** and **z** so determined satisfy (1-9). Define $\gamma_1 := m_1/\delta_1$ and $\gamma_2 := m_2/\delta_2$. By $x \underset{m}{\leftarrow} ax+b \equiv 0$ we define x to be the smallest non-negative solution of the congruence $ax+b \underset{m}{\equiv} 0$.

$$x_1 = \frac{N}{\delta_1\delta_2}$$

$$y_2 = \delta_1\delta_2$$

$$y_1 = \eta_1 + \gamma_1\eta_2,$$

where

$$\eta_1 \underset{m_1}{\leftarrow} \eta_1 a_{11} + y_2 a_{12} \equiv 0\,, \quad \eta_2 \underset{m_2}{\leftarrow} (\eta_1 + \gamma_1\eta_2)a_{21} + y_2 a_{22} \equiv 0$$

$$z_2 = \zeta_1 + \delta_1\zeta_2,$$

where

$$\zeta \underset{\delta_1}{\leftarrow} \zeta_1 a_{12} + a_{13} \equiv 0\,, \quad \zeta_2 \underset{\delta_2}{\leftarrow} (\zeta_1 + \delta_1\zeta_2)a_{22} + a_{23} \equiv 0$$

$$z_1 = \xi_1 + \gamma_1\xi_2, \tag{1-10}$$

where

$$\xi_1 \underset{m_1}{\leftarrow} \xi_1 a_{11} + z_2 a_{12} + a_{13} \equiv 0\,,$$

$$\xi_2 \underset{m_2}{\leftarrow} (\xi_1 + \gamma_1\xi_2)a_{21} + z_2 a_{22} + a_{23} \equiv 0\,.$$

A basic theorem of number theory is:* the congruence $ax+b \underset{m}{\equiv} 0$ has no integral solution x if b is not a multiple of $g := (a,m)$; if b is a multiple of g, the congruence has exactly one integral solution that satisfies $0 \le x < m/g$. This theorem shows that η_i, ζ_i, and ξ_i, $i = 1, 2$ exist and satisfy

$$0 \le \eta_i < \gamma_i\,, \quad 0 \le \zeta_i < \delta_i\,, \quad \text{and} \quad 0 \le \xi_i < \gamma_i\,.$$

η_i, ζ_i and ξ_i can be found by hand or computer by trying consecutively for the unknown number the values $0, 1, 2, \ldots$ until a solution has been found. The congruences (1-10) ensure that **x**, **y** and **z** satisfy (1-9). It follows that the vectors **Rx**, **Ry** and **Rz** lie in G_C^p. They form a basis because $\det[\mathbf{Rx}, \mathbf{Ry}, \mathbf{Rz}] = \det[\mathbf{x}, \mathbf{y}, \mathbf{z}] = x_1 \,.\, y_2 \,.\, 1 = N$.

If $(a_{11}, N) = 1$, which is fulfilled in the majority of examples in Table 1, our algorithm simplifies considerably:

$$x_1 = N$$

$$y_2 = 1\,, \quad y_1 \underset{N}{\leftarrow} y_1 a_{11} + a_{12} \equiv 0$$

$$z_2 = 0\,, \quad z_1 \underset{N}{\leftarrow} z_1 a_{11} + a_{13} \equiv 0\,.$$

We give an example:

$$\mathbf{R} = \tfrac{1}{13}\begin{pmatrix} 12 & -3 & 4 \\ 4 & 12 & -3 \\ -3 & 4 & 12 \end{pmatrix}$$

$$y_1 = 10 \underset{13}{\leftarrow} 12y_1 - 3 \equiv 0\,, \quad z_1 = 4 \underset{13}{\leftarrow} 12z_1 + 4 \equiv 0\,.$$

A basis **B** for G_C^p is therefore given by

$$\mathbf{B} = \tfrac{1}{13}\begin{pmatrix} 12 & -3 & 4 \\ 4 & 12 & -3 \\ -3 & 4 & 12 \end{pmatrix}\begin{pmatrix} 13 & 10 & 4 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 12 & 9 & 4 \\ 4 & 4 & 1 \\ -3 & -2 & 0 \end{pmatrix}.$$

Table 1 gives for our example the basis matrix **B** . **U**, where

$$\mathbf{U} = \begin{pmatrix} -1 & -2 & 1 \\ 1 & 2 & -2 \\ 1 & 1 & 2 \end{pmatrix}.$$

Notice that **B** and **B** . **U** determine the same lattice because **U** has integral elements and determinant 1.

PART II

2.1 Introduction to Part II

While the terms of group theory and number theory are more appropriate for proofs of the essential mathematical relations, the methods of matrix calculations are often more convenient for the numerical procedures, especially in connexion with calculations on grain-boundary structures by means of a computer.

In § 2.2 the 0-lattice method for determining the lattices Λ_C^p, Λ_C^b and Λ_C^f in either orthonormal coordinates of Λ_1^p or in the crystal coordinates of Λ_1^b and Λ_1^f is developed. § 2.3 describes the corresponding lattices Λ_D^p, Λ_D^b and Λ_D^f and their relation to the CSL's. In § 2.4 the body and face centring of Λ_D^p and Λ_C^p is explained. § 2.5 gives a method to determine the planar density of coincidence sites and § 2.6 gives a comment on Table 1. The numerical data in the Table have been calculated by the 0-lattice method on a time-sharing computer IBM/370.

2.2 0-Lattice method for calculating the CSL's Λ_C^p, Λ_C^b, and Λ_C^f

Since the 0-lattice is defined as the lattice of all the coincidences of 'equivalent' positions (positions with the same coordinates within the interpenetrating unit cells), the CSL which consists of the coincidences of lattice points is contained as a sublattice in every 0-lattice for a given relative orientation of the two crystal lattices. Hence we can calculate a convenient 0-lattice and compose the unit cell of the CSL from 0-lattice unit cells.

The method for calculating the 0-lattice is given in detail by Bollmann (1970). First, a point-to-point relation between the two lattices has to be formulated.

$$\mathbf{x}^{(2)} = \mathbf{A}\mathbf{x}^{(1)}. \tag{2-1}$$

By the choice of the transformation **A** the 'equivalence' of points is defined. The 0-lattice is given by the solution of the equation:

$$(\mathbf{I} - \mathbf{A}^{-1})\mathbf{x}^{(0)} := \mathbf{T}\mathbf{x}^{(0)} = \mathbf{b}^{(L)}; \tag{2-2}$$

* *Cf.*, *e.g.*, p. 11 of Dickson (1957).

$\mathbf{I}$ = identity, unit transformation;

$\mathbf{b}^{(L)}$ are lattice vectors of the *b*-lattice which is composed of all the translation vectors of lattice 1 and which is in structure and orientation identical with lattice 1 but has another meaning. Equation (2-2) can be understood as an imaging relation between the *b*-lattice and the interpenetrating crystal lattices.

In all the numerical procedures the following points have to be stated beforehand:

1. The crystal lattice to be studied [primitive cubic (p.c.), body-centred cubic (b.c.c.) or face-centred cubic (f.c.c.)].

2. The coordinate system in which the results are to be represented, the orthonormal system of the p.c. unit of crystal 1, or a crystal coordinate system of the b.c.c. or f.c.c. structure (*e.g.* rhombohedral for f.c.c.).

We describe the procedure in crystal coordinates marked by (′) which also includes the p.c. case in its 'crystal coordinate system'. The advantage of the crystal coordinate system is that the matrix $\mathbf{C}'$, which contains the unit vectors of the CSL as column vectors, always consists of integral coefficients. The following expressions have to be calculated:

$$(\mathbf{I}-\mathbf{A}'^{-1}) := \mathbf{T}' = (\mathbf{I}-\mathbf{U}\mathbf{S}^{-1}\mathbf{R}^{-1}\mathbf{S}) \qquad (2\text{-}3)$$

$$\det(\mathbf{T}') = \frac{n}{\Sigma} \qquad (2\text{-}4)$$

$$\mathbf{X}'^{(0)} = \mathbf{T}'^{-1}. \qquad (2\text{-}5)$$

Transformed to orthonormal coordinates (*e.g.* for plotting the results):

$$\mathbf{X}^{(0)} = \mathbf{S}\mathbf{T}'^{-1}; \qquad (2\text{-}6)$$

$\mathbf{R}$ is the rotation matrix of the coincidence orientation under investigation expressed in the orthonormal coordinate system of a p.c. lattice 1 [equation (1-1)].

$\mathbf{S}$ is the structure matrix which contains as column vectors the unit vectors of the crystal coordinate system expressed in the orthonormal coordinates of the p.c. lattice 1. In the p.c. structure $\mathbf{S}=\mathbf{I}$ ($\mathbf{I}$ = identity = unit matrix).

n is an integral number, which indicates the number of 0-lattice units per CSL unit.

$\mathbf{X}^{(0)}$ is represented here as a matrix, the three column vectors of which are the unit vectors of the 0-lattice. This is possible if rank $(\mathbf{T})=3$, in which case the 0-lattice is a point lattice.

According to Theorem 1, the value of Σ is equal to the number N in the rotation matrix.

$\mathbf{U}$ is a unimodular transformation which is needed in order to obtain $\det(\mathbf{T}')\neq 0$. A unimodular transformation has the property $\det(\mathbf{U})=\pm 1$ and in our case has integral coefficients. It redefines the units of the coordinate system usually by a shear transformation with a component in the direction of the axis of rotation, and so images lattice 1 onto itself.

$\mathbf{U}$ is needed for the following reason: if the relation $\mathbf{A}$ between the two crystal lattices is given by the rotation $\mathbf{R}$ alone, then rank $(\mathbf{T}')=2$ and the 0-lattice becomes a line-lattice. Hence the coincidence sites lie on parallel lines and a basis of the CSL has to be found from these points. This task becomes easier if the 0-lattice is a point lattice, *i.e.* if rank $(\mathbf{T}')=3$ and this is achieved by a convenient choice of $\mathbf{U}$.

The next step is the determination of a basis matrix $\mathbf{C}'$ for the CSL from $\mathbf{X}'^{(0)}$ ($\mathbf{C}'$ = CSL-matrix in crystal coordinates). As already mentioned, the coefficients of $\mathbf{C}$ are integers. $\mathbf{C}'$ is determined in two steps: first by operating on the columns of $\mathbf{X}'^{(0)}$ such that its determinant ($=\Sigma/n$) remains unchanged* and that two columns become integers and then, in the second step, the remaining column can be multiplied by n whereby the determinant becomes Σ.† The column vectors of the matrix thus determined $\mathbf{C}'$ are a basis of the CSL in crystal coordinates.

By further operating on the column vectors of $\mathbf{C}'$ the unit cell of the CSL can be reshaped such that its form is most cube-like and so its vectors acquire the shortest length. The $\mathbf{C}^p$ matrices in the Table (CSL column) are reshaped such that the first unit vector has a component in the direction of the axis of rotation and in most cases lies in this axis, and the two other unit vectors are, as far as possible, perpendicular to it. The sequence of unit vectors is always chosen right-handed, *i.e.* the determinant of $\mathbf{C}^p$ is positive.

It is to be mentioned that by the 0-lattice method the matrices $\mathbf{C}^b$ and $\mathbf{C}^f$ can be determined directly without passing through $\mathbf{C}^p$.

2.2.1 *Example for the calculation of the matrix* $\mathbf{C}^p$

Data from Table 1

$\Sigma=13$ ([111]-axis $\theta=27{\cdot}79°$), p.c. lattice

$$\mathbf{R}=\tfrac{1}{13}\begin{pmatrix}12 & -3 & 4\\ 4 & 12 & -3\\ -3 & 4 & 12\end{pmatrix}.$$

$\mathbf{R}^{-1}=\mathbf{R}^T$ as $\mathbf{R}$ is an orthogonal transformation. Chosen $\mathbf{U}$:

$$\mathbf{U}=\begin{pmatrix}1 & 0 & 1\\ 0 & 1 & 0\\ 0 & 1 & 1\end{pmatrix}.$$

---

* The determinant of a matrix (*i.e.* the volume given by the three column vectors) is conserved if multiples of other column vectors are added to a column vector. The determinant changes its sign (change from right-hand to left-hand system) if one column vector changes its sign or if the sequence of two column vectors is inverted. The determinant increases by a factor n if one column vector is multiplied by n. All these operations correspond geometrically to new choices of unit cells within a lattice.

With respect to the value of the determinant, the same operations could be carried out with row vectors, the structure of the lattice, however, would then be changed.

† It may be that n [from $\det(\mathbf{T}')=n/\Sigma$] can be expressed as a product of several factors. In this case $\mathbf{X}^{(0)}$ may be such that different column vectors have to be multiplied by different factors in order to obtain a unit cell of the CSL (with integer coefficients and the determinant Σ).

For the centred lattices **S** can be chosen:

$$\mathbf{S}^b=\begin{pmatrix}\frac{1}{2} & -\frac{1}{2} & 0\\ \frac{1}{2} & \frac{1}{2} & 0\\ \frac{1}{2} & \frac{1}{2} & 1\end{pmatrix} \quad \text{and} \quad \mathbf{S}^f=\begin{pmatrix}\frac{1}{2} & \frac{1}{2} & 0\\ 0 & \frac{1}{2} & \frac{1}{2}\\ \frac{1}{2} & 0 & \frac{1}{2}\end{pmatrix}$$

$$\mathbf{T}'=\tfrac{1}{13}\begin{pmatrix}-3 & -1 & -9\\ 3 & 1 & -4\\ -1 & -9 & -3\end{pmatrix}$$

$$\mathbf{X}^{(0)}=\left(\begin{array}{c|c|c} -\frac{3}{2} & 3 & \frac{1}{2}\\ \frac{1}{2} & 0 & -\frac{3}{2}\\ -1 & -1 & 0\end{array}\right).$$

Since $n=2$ this 0-lattice unit is half a CSL unit. In order to obtain a complete CSL unit we add the third column to the first and then double the third column.

$$\mathbf{C}^p=\left(\begin{array}{c|c|c} -1 & 3 & 1\\ -1 & 0 & -3\\ -1 & -1 & 0\end{array}\right).$$

This form can be reshaped to the form given in Table 1.

2.3 Determination of the DSC lattice

As shown in § 1.4.2 the DSCL for the p.c. structure is the reciprocal lattice of the CSL. $\mathbf{D}^p$ matrix with the unit vectors of the DSCL as column vectors can be determined by

$$\mathbf{D}^p=[(\mathbf{C}^p)^{-1}]^T, \qquad (2\text{-}7)$$

T=transpose.

There is also a direct method for determining $\mathbf{D}^p$, $\mathbf{D}^b$ and $\mathbf{D}^f$ described by Warrington & Bollmann (1972). (In that paper the D-matrix is called $\mathbf{D}^{(2-SC)}$.)

2.4 Body centring and face centring

Since in Table 1 only the $\mathbf{C}^p$ and $\Sigma\,.\,\mathbf{D}^p$ matrices are given we describe here the transformation to the $\mathbf{C}^b$, $\mathbf{D}^b$ and $\mathbf{C}^f$, $\mathbf{D}^f$ matrices. As was shown in § 1.3.1 there are four classes of column vectors of the matrices $\mathbf{C}^p$ and $\Sigma\,.\,\mathbf{D}^p$ with respect to the number of odd and even components. A vector of class 0 halved leads to lattice points of A_1^p (integer coordinates), one of class 1 halved leads to centres of cube edges, one of class 2 to face centres, and a vector of class 3 to body centres.

Hence, for face centring two columns of class 2 have to be halved and for body centring one column of class 3. The form in which the matrices are given in Table 1 does not always contain the needed class of columns. Hence, such columns have to be made of combinations of columns in the matrix, which leave the determinant unchanged, and then the corresponding new columns have to be halved. This can be done by constructing a matrix $\mathbf{Z}^b$ or $\mathbf{Z}^f$ such that

$$\mathbf{C}^b=\mathbf{C}^p\mathbf{Z}^b \quad (\mathbf{C}^f=\mathbf{C}^p\mathbf{Z}^f) \qquad (2\text{-}8)$$

and correspondingly

$$\Sigma\,.\,\mathbf{D}^b=\Sigma\,.\,\mathbf{D}^p\mathbf{Z}^b \quad (\Sigma\,.\,\mathbf{D}^f=\Sigma\,.\,\mathbf{D}^p\mathbf{Z}^f)\,. \qquad (2\text{-}9)$$

The **Z** matrices depend on the odd–even structure of the attributed **C** or $\Sigma\,.\,\mathbf{D}$ matrices.

We show the procedure on the example $\Sigma=13$ rotation around the [111] axis by 27·79°

$$\mathbf{C}^p=\begin{pmatrix}1 & -2 & 2\\ 1 & 1 & -2\\ 1 & 2 & 1\end{pmatrix} \quad \Sigma\,.\,\mathbf{D}^p=\begin{pmatrix}5 & -3 & 1\\ 6 & -1 & -4\\ 2 & 4 & 3\end{pmatrix}.$$

The odd–even structures are

$$\mathbf{C}^p=\begin{pmatrix}d & e & e\\ d & d & e\\ d & e & d\end{pmatrix} \quad \Sigma\,.\,\mathbf{D}^p=\begin{pmatrix}d & d & d\\ e & d & e\\ e & e & d\end{pmatrix}^{*}.$$

For body centring **C** we have to halve the first column and leave the two other columns unchanged. Hence $\mathbf{Z}^b$ here becomes

$$\mathbf{Z}_C^b=\begin{pmatrix}\frac{1}{2} & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{pmatrix}.$$

The determinant of $\mathbf{Z}^b$ has to be $\frac{1}{2}$, as the volume of the $\mathbf{C}^p$ unit cell is halved by body centring. For the face centring of $\mathbf{C}^p$, first two columns with two odd components have to be produced before they can be halved. This can be done in the following way,

$$\mathbf{Z}_C^f=\begin{pmatrix}1 & \frac{1}{2} & \frac{1}{2}\\ 0 & \frac{1}{2} & 0\\ 0 & 0 & \frac{1}{2}\end{pmatrix}.$$

The columns of $\mathbf{Z}_C^f$ show that the first column of $\mathbf{C}^f$ equals the first column of $\mathbf{C}^p$, the second column of $\mathbf{C}^f$ is the first and the second column of $\mathbf{C}^p$ added and halved, and correspondingly the third column. The determinant of $\mathbf{Z}^f$ has to be $\frac{1}{4}$ since by face centring the volume of $\mathbf{C}^p$ is divided by 4. The corresponding **Z** matrices for $\Sigma\,.\,\mathbf{D}$ are:

$$\mathbf{Z}_D^b=\begin{pmatrix}\frac{1}{2} & 0 & 0\\ \frac{1}{2} & 1 & 0\\ \frac{1}{2} & 0 & 1\end{pmatrix} \quad \text{and} \quad \mathbf{Z}_D^f=\begin{pmatrix}1 & 0 & 0\\ 0 & \frac{1}{2} & 0\\ 0 & 0 & \frac{1}{2}\end{pmatrix}.$$

To summarize the construction of the **Z** matrix, the ith column in the **Z** matrix refers to the ith column of the new, centred matrix, and the coefficients in that column, in their respective row positions, refer to the columns of the old, non-centred matrix, which have to be multiplied by these coefficients and added in order to obtain the new column.

---

* The calculation rules of the odd–even algebra obviously are:

±	d	e
d	e	d
e	d	e

×	d	e
d	d	e
e	e	e

The centred matrices then become

$$\mathbf{C}^b=\begin{pmatrix}\frac{1}{2} & -2 & 2\\ \frac{1}{2} & 1 & -2\\ \frac{1}{2} & 2 & 1\end{pmatrix} \qquad \mathbf{C}^f=\begin{pmatrix}1 & \frac{1}{2} & \frac{3}{2}\\ 1 & 1 & -\frac{1}{2}\\ 1 & \frac{3}{2} & 1\end{pmatrix}$$

$$\mathbf{D}^b=\tfrac{1}{13}\begin{pmatrix}\frac{3}{2} & -3 & 1\\ \frac{1}{2} & -1 & -4\\ \frac{9}{2} & 4 & 3\end{pmatrix} \qquad \mathbf{D}^f=\tfrac{1}{13}\begin{pmatrix}5 & -\frac{3}{2} & \frac{1}{2}\\ 6 & -\frac{1}{2} & -2\\ 2 & 2 & \frac{3}{2}\end{pmatrix}.$$

The thus-centred unit cells are still represented in the orthonormal coordinate system of Λ_1^p.

2.5 Planar density of coincidence sites

For the study of grain boundaries it is of importance to know the density of coincidence sites within the boundary surface, as only the density in this surface may have physical significance, in contrast to the density in space. We calculate the planar density assuming that a curved or faceted surface can be composed of planar parts.

Suppose the indices of a plane ($h_i^{(\mathrm{cub})}$) are given in the cubic system and we need to know the ratios: number of atomic sites per coincidence site and number of coincidences sites per unit surface. The crystal may have a p.c., b.c.c. or f.c.c. lattice. It is convenient for this purpose to express the vector $\mathbf{h}_i^{(\mathrm{cub})}$ in the coordinate system of the reciprocal coincidence-site lattice as well as in the reciprocal crystal system. The length of a vector in a reciprocal lattice [with no common factor of its (integer) coordinates] is the inverse of the layer spacing of the corresponding crystal lattice planes and CSL planes respectively. The volume per lattice point is given by the volume of the unit cell (determinant of matrices **S** or **C**). From here the surface per lattice point in the chosen boundary plane is determined. The coordinate transformations needed are shown in Fig. 2.

The procedure is the following:

The vector $\mathbf{h}^{(\mathrm{cub})}$ is transformed into the coordinate system of the reciprocal CSL (r . CSL)

$$\mathbf{h}^{(r.\mathrm{CSL})}=\mathbf{C}^T\mathbf{h}^{(\mathrm{cub})} \tag{2-10}$$

and correspondingly to the reciprocal crystal system (r . crst) (*e.g.* rhombohedral for f.c.c.).

$$\mathbf{h}^{(r.\mathrm{crst})}=\mathbf{S}^T\mathbf{h}^{(\mathrm{cub})}. \tag{2-11}$$

In general the resulting representations $\mathbf{h}^{(r.\mathrm{CSL})}$ and $\mathbf{h}^{(r.\mathrm{crst})}$ do not have integer coordinates. Hence they have to be multiplied by a factor such that their coordinates become integers with no common factor. The thus-corrected **h** vectors will be marked by a prime. The corresponding layer spacing in the CSL and in the crystal then is:

$$d^{(\mathrm{CSL})}=\frac{1}{|\mathbf{h}'^{(r.\mathrm{CSL})}|} \qquad d^{(\mathrm{crst})}=\frac{1}{|\mathbf{h}'^{(r.\mathrm{crst})}|}. \tag{2-12}$$

The length of the vector $\mathbf{h}'$ is given by means of the metric tensor **G** by:

$$|\mathbf{h}'^{(\alpha)}|=[(\mathbf{h}'^{(\alpha)})^T\mathbf{G}^{(\alpha)}\mathbf{h}'^{(\alpha)}]^{1/2} \tag{2-13}$$

with (α) either (r . CSL) or (r . crst) and

$$\mathbf{G}^{(r.\mathrm{CSL})}=(\mathbf{C}^T\mathbf{C})^{-1}=\mathbf{C}^{-1}(\mathbf{C}^T)^{-1} \tag{2-14}$$

and

$$\mathbf{G}^{(r.\mathrm{crst})}=(\mathbf{S}^T\mathbf{S})^{-1}=\mathbf{S}^{-1}(\mathbf{S}^T)^{-1}. \tag{2-15}$$

The volume per coincidence site is given by the layer spacing d of the CSL times the surface f per coincidence site:

$$d\,.\,f=\frac{1}{|\mathbf{h}'|}\,.\,f=v\,. \tag{2-16}$$

A similar formula applies to the density of lattice sites. Since the volume v equals $|\mathbf{C}|$, the determinant of **C**, or $|\mathbf{S}|$ respectively, the ratio (in the plane **h**) of the number of crystal-lattice points per coincidence site is given by

$$\frac{n^{(\mathrm{crst})}}{n^{(\mathrm{CSL})}}=\frac{|\mathbf{C}|\,.\,|\mathbf{h}'^{(r.\mathrm{CSL})}|}{|\mathbf{S}|\,.\,|\mathbf{h}'^{(r.\mathrm{crst})}|} \tag{2-17}$$

and the number of coincidence sites per unit surface (Å^2)

$$n^{(\mathrm{CSL})}(\text{Å}^{-2})=\frac{1}{a^2\,.\,|\mathbf{C}|\,.\,|\mathbf{h}'^{(r.\mathrm{CSL})}|} \tag{2-18}$$

with a the lattice constant of the cubic system in Å.

The ratio $n^{(\mathrm{crst})}/n^{(\mathrm{CSL})}$ can acquire the value Σ or one of its factors down to the value 1.

As an example it can be shown that the $\Sigma=3$ case, the (111) plane, is greatly preferred in the f.c.c. structure (twin boundary) as there $n^{(\mathrm{crst})}/n^{(\mathrm{CSL})}=1$ and $n^{(\mathrm{CSL})}/a^2=2\cdot 31/a^2$.

2.6 Comment on Table 1

The columns of Table 1 give the following information:

1. Σ value, axis of rotation, angle of rotation.
2. Σ times the rotation matrix.
3. Matrix that determines the coincidence site lattice Λ_C^p (column vectors are the unit vectors of the CSL).

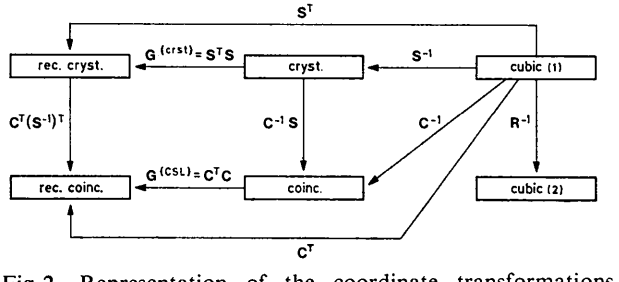

Fig. 2. Representation of the coordinate transformations needed for the determination of the planar density of coincidence sites.

4. Matrix that determines Σ times the DSC lattice Λ_D^p.

5. A number that gives the Bravais class of Λ_C^p and Λ_D^p according to the following list:

number	Bravais class of Λ_C^p and Λ_D^p
1	hexagonal
2	rhombohedral
3	tetragonal P
4	orthorhombic P
5	orthorhombic C
6	monoclinic P
7	monoclinic C.

Table 1. *Coincident-site lattices*

The explanation of the Table is given in § 2.6.

Σ [hkl] θ°	Σ·ROT			CSL			Σ·DSCL			BC
3	2	-1	2	1	1	-1	1	1	-1	1
[111]	2	2	-1	1	0	1	1	1	2	
60.00°	-1	2	2	1	-1	0	1	-2	-1	
5	5	0	0	1	0	0	5	0	0	3
[100]	0	4	-3	0	1	-2	0	1	-2	
36.86°	0	3	4	0	2	1	0	2	1	
7	6	-2	3	1	2	-1	2	2	-1	2
[111]	3	6	-2	1	0	2	1	1	3	
38.21°	-2	3	6	1	-1	0	4	-3	-2	
9	8	1	4	1	-2	0	5	-2	1	5
[110]	1	8	-4	1	2	-1	4	2	-1	
38.94°	-4	4	7	0	1	2	2	1	4	
11	9	2	6	1	1	1	7	1	3	5
[110]	2	9	-6	1	-1	-2	4	-1	-3	
50.47°	-6	6	7	0	3	-1	-1	3	-2	
13	13	0	0	1	0	0	13	0	0	3
[100]	0	12	-5	0	3	2	0	3	2	
22.61°	0	5	12	0	-2	3	0	-2	3	
13	12	-3	4	1	-2	2	5	-3	1	2
[111]	4	12	-3	1	1	-2	6	-1	-4	
27.79°	-3	4	12	1	2	1	2	4	3	
15	14	2	5	2	-1	0	6	-3	1	5
[210]	2	11	-10	1	2	0	3	6	-2	
48.18°	-5	10	10	0	1	3	0	0	5	
17	17	0	0	1	0	0	17	0	0	3
[100]	0	15	-8	0	1	4	0	1	4	
28.07°	0	8	15	0	-4	1	0	-4	1	
17	12	-1	12	2	-3	0	4	-3	2	5
[221]	9	12	-8	2	2	-1	3	2	-7	
61.92°	-8	12	9	1	2	1	3	2	10	
19	18	1	6	1	-3	1	9	-3	1	5
[110]	1	18	-6	1	3	0	10	3	-1	
26.52°	-6	6	17	0	1	3	-3	1	6	
19	15	-6	10	1	3	-2	6	3	-2	2
[111]	10	15	-6	1	0	3	4	2	5	
46.82°	-6	10	15	1	-2	0	9	-5	-3	

Σ [hkl] θ°	Σ·ROT			CSL			Σ·DSCL			BC
21	20	-4	5	1	-3	2	7	-4	1	1
[111]	5	20	-4	1	1	-3	7	-1	-5	
21.78°	-4	5	20	1	2	1	7	5	4	
21	19	-4	8	2	1	0	10	1	-4	5
[211]	8	16	-11	0	-4	-1	2	-4	-5	
44.41°	-4	13	16	-1	2	-2	-1	2	-8	
23	22	-3	6	3	1	0	8	-1	3	7
[311]	6	18	-13	0	3	1	-2	6	5	
40.45°	-3	14	18	-1	-2	2	1	-3	9	
25	25	0	0	1	0	0	25	0	0	3
[100]	0	24	-7	0	4	3	0	4	3	
16.26°	0	7	24	0	-3	4	0	-3	4	
25	20	0	15	2	1	-2	5	5	-5	7
[331]	9	20	-12	1	2	3	1	6	4	
51.68°	-12	15	16	2	-1	1	7	-8	3	
27	25	2	10	1	-2	1	16	-5	1	5
[110]	2	25	-10	1	3	-1	11	5	-1	
31.59°	-10	10	23	0	1	5	-1	2	5	
27	26	2	7	2	-2	-1	11	-1	-3	7
[210]	2	23	-14	1	2	3	5	2	6	
35.43°	-7	14	22	0	-3	1	-4	-7	6	
29	29	0	0	1	0	0	29	0	0	3
[100]	0	21	-20	0	5	-2	0	5	-2	
43.60°	0	20	21	0	2	5	0	2	5	
29	24	-3	16	1	-1	-4	6	-7	-4	6
[221]	11	24	-12	2	0	3	10	-2	3	
46.40°	-12	16	21	-1	-2	2	-3	-11	2	
31	30	-5	6	1	-4	2	9	-5	1	2
[111]	6	30	-5	1	1	-4	8	-1	-6	
17.90°	-5	6	30	1	2	1	14	6	5	
31	27	6	14	1	2	-2	5	11	-2	7
[320]	6	22	-21	3	-1	2	8	-1	3	
54.50°	-14	21	18	1	-1	-3	2	-8	-7	
33	32	1	8	1	-4	1	16	-4	1	5
[110]	1	32	-8	1	4	0	17	4	-1	
20.05°	-8	8	31	0	1	4	-4	1	8	

Σ [hkl] θ°	Σ·ROT			CSL			Σ·DSCL			BC
33	32	-4	7	3	-1	-1	9	-1	-5	5
[311]	7	28	-16	1	4	1	3	7	2	
33.56°	-4	17	28	1	-1	2	3	-4	13	
33	25	8	20	1	2	2	19	2	5	5
[110]	8	25	-20	1	-2	-3	14	-2	-5	
58.99°	-20	20	17	0	5	-2	-2	5	-4	
35	33	-6	10	2	-1	1	13	-8	1	5
[211]	10	30	-15	1	1	-5	5	5	-5	
34.05°	-6	17	30	1	2	3	4	11	3	
35	30	-1	18	1	-2	-2	7	-6	-8	5
[331]	10	30	-15	0	4	-3	0	5	-5	
43.23°	-15	18	26	2	1	1	14	3	4	
37	37	0	0	1	0	0	37	0	0	3
[100]	0	35	-12	0	6	-1	0	6	-1	
16.92°	0	12	35	0	1	6	0	1	6	
37	36	3	8	3	2	2	9	1	4	7
[310]	3	28	-24	1	-1	-2	10	-3	-12	
43.14°	-8	24	27	0	4	-1	-2	8	-5	
37	28	-12	21	1	3	0	16	7	4	2
[111]	21	28	-12	1	-4	3	12	-4	3	
50.57°	-12	21	28	1	0	-4	9	-3	-7	
39	35	-10	14	1	3	1	13	7	5	1
[111]	14	35	-10	1	-4	3	13	-5	2	
32.20°	-10	14	35	1	1	-4	13	-2	-7	
39	34	-2	19	3	2	0	9	6	1	7
[321]	14	29	-22	2	-3	0	6	-9	5	
50.13°	-13	26	26	1	-1	-3	0	0	-13	
41	41	0	0	1	0	0	41	0	0	3
[100]	0	40	-9	0	5	4	0	5	4	
12.68°	0	9	40	0	-4	5	0	-4	5	
41	39	4	12	2	-1	-2	14	-1	-6	6
[210]	4	33	-24	1	2	2	13	2	12	
40.88°	-12	24	31	0	-6	1	2	-6	5	
41	32	9	24	1	4	-2	19	4	-3	5
[110]	9	32	-24	1	-4	1	22	-4	3	
55.88°	-24	24	23	0	-3	-4	-4	-3	-8	

Σ [hkl] θ°	Σ·ROT			CSL			Σ·DSCL			BC
43	42	-6	7	1	2	-4	17	-1	-7	2
[111]	7	42	-6	1	3	2	10	7	6	
15.18°	-6	7	42	1	-4	3	16	-6	1	
43	42	2	9	2	1	1	19	1	4	7
[210]	2	39	-18	1	-3	-4	5	-2	-8	
27.91°	-9	18	38	0	4	-1	-1	9	-7	
43	30	-7	30	3	0	-5	6	-3	-5	5
[332]	25	30	-18	3	1	3	5	19	3	
60.77°	-18	30	25	2	-1	3	5	-24	3	
45	44	-5	8	3	0	2	11	1	6	7
[311]	8	40	-19	1	-5	-1	2	-8	-3	
28.62°	-5	20	40	1	1	-2	10	5	-15	
45	40	-5	20	2	-5	0	10	-5	0	4
[221]	13	40	-16	2	4	-1	10	4	-9	
36.87°	-16	20	37	1	2	2	5	2	18	
45	35	-4	28	2	-4	1	6	-7	5	7
[221]	20	35	-20	2	1	-1	15	5	-10	
53.13°	-20	28	29	1	3	3	3	4	10	
47	42	-2	21	3	0	-2	11	-5	-7	7
[331]	11	42	-18	3	1	4	4	11	6	
37.07°	-18	21	38	1	-2	3	2	-18	3	
47	43	6	18	3	1	0	15	2	-5	7
[320]	6	38	-27	-1	0	-3	1	-3	-16	
43.66°	-18	27	34	-1	5	-1	-3	9	1	
49	40	-15	24	1	-4	4	17	-5	3	2
[111]	24	40	-15	1	1	-4	20	-3	-8	
43.57°	-15	24	40	1	4	1	12	8	5	
49	48	-4	9	4	0	1	11	-1	5	7
[511]	9	36	-32	0	5	1	-1	9	4	
43.57°	-4	33	36	-1	-1	2	-5	-4	20	
49	41	-12	24	3	0	2	15	-3	2	6
[322]	24	36	-23	1	1	-6	4	9	-6	
49.23°	-12	31	36	0	2	3	-2	20	3	

Because the symmetry elements are present in both lattices (24 rotations if mirror imaging is excluded) many congruent CSL's can be produced by rotations around different axes with different angles θ. The rotation matrices with axes within the standard stereographic triangle ([100], [110], [111]) up to $\Sigma=25$ are given by Warrington & Bufalini (1971). Before that, Pumphrey & Bowkett (1971) gave a list containing the axis of rotation, the rotation angle and the Σ value up to $\Sigma=19$. For a given Σ value there may exist several different structures of the CSL (and DSCL) corresponding to different solutions of equations (1-2). For every possible structure of the CSL and DSCL* Table 1 shows the rotation with lowest θ (disorientation) and the axis in the standard triangle. Every CSL and DSCL is represented by the most cube-like right-handed unit cell such that the first column vector has a component in the direction of the rotation axis and the other two vectors are as far as possible perpendicular to that axis.

The Bravais class of Λ_C^p has been determined by a method described by Mighell, Santoro & Donnay in *International Tables for X-ray Crystallography* (1969). Once the Bravais class of Λ_C^p is known, we also know the Bravais class of Λ_D^p because it is known [*Cf.*, *e.g.*, p. 13 of *International Tables for X-ray Crystallography* (1969)] that reciprocal lattices belong to the same Bravais class unless one lattice is f.c.c. or face-centred orthorhombic, in which cases the other is b.c.c. or body-centred orthorhombic.

We make the following observations: up to $\Sigma=49$ there exists a Λ_C^p (and Λ_D^p) that has:

(1) (at least) tetragonal symmetry if and only if $\Sigma=m^2+n^2$, where m and n are integers without a common divisor. The symmetry is even cubic if and only if $\Sigma=1$.

(2) (at least) rhombohedral symmetry if and only if $\Sigma=m^2+mn+n^2$, where m and n are integers without a common divisor. The symmetry is even hexagonal if and only if Σ is a multiple of 3.

APPENDIX

The aim of this Appendix is to prove $V_C^p=NV_1^p$, where V_1^p and V_C^p are the volumes of primitive cells of a p.c.

* Ishida & McLean (1972) determined the Burgers vectors of boundary dislocations for the b.c.c. and f.c.c. lattices up to $\Sigma=19$. Unfortunately their derivation and data contain several errors. Acton & Bevis (1971) listed CSL matrices for the primitive cubic lattices up to $\Sigma=31$.

lattice 1 and of the CSL obtained from it by a rotation matrix with denominator N. The proof makes use of three lemmas of a number-theoretical nature. The following notation has been found convenient for stating and proving these lemmas. $\mathscr{Z}$ stands for the set of all integers, $\mathscr{Z}^3$ for the set of all vectors that have all three components integral in the orthonormal crystal coordinate system of Λ_1^p. We denote the largest common divisor of integers $a_1, \ldots, a_n$ by $(a_1, \ldots, a_n)$. $a \underset{n}{\equiv} b$ states that $a-b$ is an (integral) multiple of n. We write $\mathbf{A}$ for the vector $\{A_1, A_2, A_3\}$, $\mathbf{A} \,.\, \mathbf{B}$ for the scalar product and $\mathbf{A} \times \mathbf{B}$ for the vector product of $\mathbf{A}$ and $\mathbf{B}$:

$$\mathbf{A} \,.\, \mathbf{B} = A_1B_1 + A_2B_2 + A_3B_3$$
$$\mathbf{A} \times \mathbf{B} = \{A_2B_3 - A_3B_2, A_3B_1 - A_1B_3, A_1B_2 - A_2B_1\} .$$

$\mathbf{r}_i$ stands for the ith row of the rotation matrix $\mathbf{R}$ and $\mathbf{a}_i := N\mathbf{r}_i$.

Lemma 1. *N divides every component of* $\mathbf{a}_2 \times \mathbf{a}_3$, $\mathbf{a}_3 \times \mathbf{a}_1$, *and* $\mathbf{a}_1 \times \mathbf{a}_2$

Proof: Because $\mathbf{r}_1$, $\mathbf{r}_2$ and $\mathbf{r}_3$ define a right-handed orthonormal coordinate system, we have $\mathbf{r}_1 \times \mathbf{r}_2 = \mathbf{r}_3$ and $\mathbf{a}_1 \times \mathbf{a}_2 = N\mathbf{a}_3$. Since $\mathbf{a}_3$ has integral components, the components of $\mathbf{a}_1 \times \mathbf{a}_2$ must be divisible by N. The lemma follows if we take into account that the above argument can be repeated with 1,2,3 cyclically permuted.

Define $\alpha := (a_{11}, a_{12}, N)$, $\beta := (a_{21}, a_{22}, N)$, $\delta := (\alpha, \beta)$.

Lemma 2. $\delta = 1$

Proof: $a_{13}^2 = N^2 - a_{11}^2 - a_{12}^2 \underset{\alpha^2}{\equiv} 0$ shows that the integer a_{13} is an integral multiple of α. Similarly one shows that a_{23} is a multiple of β. From $a_{3i}^2 = N^2 - a_{1i}^2 - a_{2i}^2 \underset{\delta^2}{\equiv} 0$ for $i = 1,2,3$ it follows that a_{3i}, $i = 1,2,3$ are multiples of δ. Therefore N and the nine matrix elements a_{ij} have a common divisor δ, whence $\delta = 1$.

Lemma 3. If $A_1, A_2, A_3, m \in \mathscr{Z}$, $(A_1, A_2, m) = 1$,* then the solutions $\mathbf{x} \in \mathscr{Z}^3$ of $\mathbf{A} \,.\, \mathbf{x} \underset{m}{\equiv} 0$ are given by $\mathbf{x} \underset{m}{\equiv} \mathbf{A} \times \mathbf{y}$, $\mathbf{y} \in \mathscr{Z}^3$ [*i.e.* $\mathbf{x} \in \mathscr{Z}^3$ is a solution if and only if there exists $\mathbf{y} \in \mathscr{Z}^3$ such that each component of $\mathbf{x}$ differs from the corresponding component of $\mathbf{A} \times \mathbf{y}$ by a multiple of m].

Proof: (1) Assume $\mathbf{y} \in \mathscr{Z}^3 \Rightarrow \mathbf{A} \,.\, \mathbf{x} \underset{m}{\equiv} \mathbf{A} \,.\, (\mathbf{A} \times \mathbf{y}) = 0$, *i.e.* $\mathbf{A} \,.\, \mathbf{x} \underset{m}{\equiv} 0$.

(2) Assume $\mathbf{x} \in \mathscr{Z}^3$ satisfies $\mathbf{A} \,.\, \mathbf{x} \underset{m}{\equiv} 0$. Let m_1 be the largest divisor of m such that $(m_1, A_1) = 1$ and put $m_2 := m/m_1$. Notice that $(m_1, m_2) = (m_2, A_2) = 1$. There exist integers T_1, T_2 such that $T_1A_1 \underset{m_1}{\equiv} 1$ and $T_2A_2 \underset{m_2}{\equiv} 1$.

A classical result of number theory, called the Chinese remainder theorem (see, *e.g.*, Dickson, 1957), states that there exist integers y_1, y_2, y_3 satisfying the following requirements and that these integers are determined uniquely up to integral multiples of m:

$$y_1 \underset{m_1}{\equiv} 0 \qquad y_2 \underset{m_1}{\equiv} T_1x_3 \qquad y_3 \underset{m_1}{\equiv} -T_1x_2$$
$$y_1 \underset{m_2}{\equiv} -T_2x_3 \qquad y_2 \underset{m_2}{\equiv} 0 \qquad y_3 \underset{m_2}{\equiv} T_2x_1 .$$

Therefore,

$$\left.\begin{aligned} x_1 &\underset{m_1}{\equiv} T_1A_1x_1 \underset{m_1}{\equiv} T_1(-A_2x_2 - A_3x_3) \\ &\underset{m_1}{\equiv} A_2y_3 - A_3y_2 \\ x_1 &\underset{m_2}{\equiv} T_2A_2x_1 \underset{m_2}{\equiv} A_2y_3 \underset{m_2}{\equiv} A_2y_3 - A_3y_2 \end{aligned}\right\} \Rightarrow x_1 \underset{m}{\equiv} A_2y_3 - A_3y_2 .$$

Similarly, we show $x_2 \underset{m}{\equiv} A_3y_1 - A_1y_3$ and $x_3 \underset{m}{\equiv} A_1y_2 - A_2y_1$, which ends the proof.

Theorem 1. $V_C^p = NV_1^p$

Proof: $V_C^p/V_1^p = \text{ord}\,(G_1^p/G_C^p)$, *i.e.* we have to determine ord (G_1^p/G_C^p), the number of elements in the factor group G_1^p/G_C^p.

Let m be the largest divisor of N such that $(m, \alpha) = 1$ and put $n := N/m$. It follows that $(m,n) = 1$ and, by Lemma 2, that $(n, \beta) = 1$. The definition of the CSL implies: $\mathbf{Rv} \in G_C^p$ if and only if $\mathbf{v} \in \mathscr{Z}^3$ and $\mathbf{Rv} \in \mathscr{Z}^3$. Consider $\mathbf{v} \in \mathscr{Z}^3$, we conclude:

$\mathbf{Rv} \in G_C^p \Leftrightarrow \mathbf{v} \in \mathscr{Z}^3$ and $\mathbf{a}_i \,.\, \mathbf{v} \underset{N}{\equiv} 0$ for $i = 1,2,3 \Leftrightarrow$ $\mathbf{v} \in \mathscr{Z}^3$ and $\mathbf{a}_i \,.\, \mathbf{v} \underset{m}{\equiv} 0$, $\mathbf{a}_i \,.\, \mathbf{v} \underset{n}{\equiv} 0$ for $i = 1,2,3$ ($\Leftrightarrow$ stands for 'if and only if').

Since $(a_{11}, a_{12}, m) = (m, \alpha) = 1$, there exists $\boldsymbol{\lambda} \in \mathscr{Z}^3$ such that $\boldsymbol{\lambda} \,.\, \mathbf{a}_1 \underset{m}{\equiv} 1$. We conclude: if G_m denotes the group of the $\mathbf{x} \in \mathscr{Z}^3$ that satisfy $\mathbf{x} \,.\, \mathbf{a}_1 \underset{m}{\equiv} 0$ then ord $(G_1^p/G_m) = m$. Take $\mathbf{x} \in G_m$:

$$\mathbf{x} \,.\, \mathbf{a}_2 \underset{m}{\equiv} (\mathbf{a}_1 \times \mathbf{y}) \,.\, \mathbf{a}_2 \equiv (\mathbf{a}_2 \times \mathbf{a}_1) \,.\, \mathbf{y} \underset{m}{\equiv} 0 .$$

(In the first step, we have used Lemma 3 and in the last Lemma 1.) Analogously we prove $\mathbf{x} \,.\, \mathbf{a}_3 \underset{m}{\equiv} 0$.

In the same way one shows that the $\mathbf{x} \in \mathscr{Z}^3$ satisfying $\mathbf{x} \,.\, \mathbf{a}_2 \underset{n}{\equiv} 0$ form a group G_n with ord $(G_1^p/G_n) = n$ and that $\mathbf{x} \,.\, \mathbf{a}_1 \underset{n}{\equiv} \mathbf{x} \,.\, \mathbf{a}_3 \underset{n}{\equiv} 0$ for $\mathbf{x} \in G_n$. We conclude: $\mathbf{Rv} \in G_C^p \Leftrightarrow \mathbf{v} \in G_m$ and $\mathbf{v} \in G_n$. The vectors $\mathbf{v}$ satisfying $\mathbf{v} \in G_m$ and $\mathbf{v} \in G_n$ form a group G, which is isomorphic with G_C^p. ord $(G_1^p/G) = m \,.\, n$ because $(m,n) = 1$. Therefore ord $(G_1^p/G_C^p) = m \,.\, n = N$.

This Appendix has largely profited from discussions with Dr M. Ojanguren.

* Lemma 3 remains true if we replace $(A_1, A_2, m) = 1$ by the weaker condition $(A_1, A_2, A_3, m) = 1$. However, we do not need this more general result.

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Instrumental Widths and Intensities in Neutron Crystal Diffractometry

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The amplitude and the shape of the quasielastic resolution function of a neutron two-axis spectrometer are calculated in the Gaussian approximation. Special attention is given to the explicitness of the formulae as well as to their absolute correctness, avoiding any unknown proportionality factors. The results are applied to the analysis of the elastic scattering of neutrons in crystals.

1. Introduction

In an experiment to analyse the angular distribution of scattered neutrons, carried out with a crystal diffractometer (two-axis spectrometer), the finite collimations, the monochromator mosaic structure and the beam-path configuration influence both the counting rate and the experimental line width. This influence should be quantitatively described by an instrumental function, the so-called resolution function.

The knowledge of the resolution function makes possible the choice of advantageous experimental conditions as well as the correct interpretation of experimental data. That is why great attention has been paid to the problem of determining the dependence of the diffractometer resolution function on all experimental factors.

The early papers in which resolution effects were considered deal with elastic-scattering experiments, their principal aim being the calculation of Bragg peak width and relative intensities for some usual experimental methods (Caglioti, Paoletti & Ricci, 1958, 1960; Caglioti & Ricci, 1962; Sailor, Foote, Landon & Wood, 1956; Willis, 1960).

In a more general treatment, Cooper & Nathans (1968*a*) have shown, also for elastic experiments, that the counting rate is given by the convolution, in the space of wave-vector transfers $\mathbf{Q}$ ($\mathbf{Q}=\mathbf{k}_i-\mathbf{k}_f$), of the scattering cross section with the resolution function

$$I(\mathbf{Q}_0)=\int \sigma(\mathbf{Q})R(\mathbf{Q})\mathrm{d}\mathbf{Q}\,.$$

$\mathbf{Q}_0$ is the nominal setting of the instrument as defined by the most probable wave vectors $\mathbf{k}_I$ and $\mathbf{k}_F$. In the Gaussian approximation, assuming that both the transmission functions of collimators and the reflectivity of the monochromator crystal are Gaussian-like functions, the elastic resolution function of the diffractometer can be written

$$R(\mathbf{Q}_0+\mathbf{X})=R_0\exp\{-\tfrac{1}{2}\sum_{i,j=1}^{3}M_{ij}X_iX_j\} \qquad (1)$$