$$P(|\alpha|) = \frac{\sqrt{1-r^2}}{\pi(1-r\cos 2\alpha)}, \quad 0 \le \alpha \le \pi \tag{11}$$

$$Pr(\alpha_0, \pi\text{-}\alpha_0) = 1 - \frac{2}{\pi}\sin^{-1}\left[\sqrt{\frac{(1+r)\sin^2\alpha_0}{1-r\cos 2\alpha_0}}\right], \quad 0 \le \alpha_0 \le \pi/2 . \tag{12}$$

Discussion of the results

The functional dependence of $Pr(\alpha_0, \pi - \alpha_0)$ on α_0 is shown in Fig. 1 for different values of r (which is a measure of the type-II degree of centrosymmetry). It is interesting to see that even when 50% of the atoms in the unit cell have a centrosymmetric configuration (*i.e.* $r \simeq 0\cdot5$) the distribution of the phase angles is much closer to the distribution expected for the ideally non-centrosymmetric case than for the ideally centrosymmetric case. It is useful to note that though $Pr(\alpha_0, \pi - \alpha_0)$ for the type-I case is a function of $(\sin\theta)/\lambda$ ($=S$, say), it is independent of S for the type-II case considered here since r is practically a constant for a given crystal.

It would be interesting to make a comparative study of the variation of $Pr(\alpha_0, \pi - \alpha_0)$ as a function of α_0 for typical non-centrosymmetric crystals with type-I and type-II degrees of centrosymmetry. We shall consider, for example, a non-centrosymmetric crystal with type-I degree of centrosymmetry having $\langle|\Delta\mathbf{r}|\rangle = 0\cdot1$ Å and a non-centrosymmetric crystal with type-II degree of centrosymmetry with $r = 0\cdot5$. Since $Pr(\alpha_0, \pi - \alpha_0)$ for the former is a function of S, we shall set $S = 0\cdot4$ Å^{-1} which is a typical value for Cu $K\alpha$ radiation. The relevant curves are shown in Fig. 2. It is seen that while for the type-II case about 55% of the reflexions have phases in the interval 30° to 150° (whatever the value of S), for the type-I case only about 20% of the reflections (for $S = 0\cdot4$ Å^{-1} and $\langle|\Delta\mathbf{r}|\rangle = 0\cdot1$ Å) have phases in the interval 30° and 150°. Thus, under the conditions stated above, the type-I case would be more difficult to refine than the type-II case.

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General Theory of Coincidence-Site Lattices, Reduced 0-Lattices and Complete Pattern-Shift Lattices in Arbitrary Crystals

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The definition of a lattice and its superlattice is given algebraically. A coincidence site lattice (CSL) is defined as an intersection lattice of any two crystal lattices, and a complete pattern-shift lattice (DSCL) as the set theoretically smallest lattice containing both crystal lattices as superlattices. In the case where the two lattices are related by a non-singular matrix (having non-zero determinant), the so-called 0-lattice may be generated from the two crystal lattices. Any translation of the 0-lattice by all the vectors of one of the crystal lattices forms a lattice, *i.e.* a reduced 0-lattice. As a result of the theory of groups and numbers, the reduced 0-lattice (abbreviated to R0L) is homomorphic to the DSCL. It is shown that the factor group of all cosets of lattice 1 in the DSCL (in the R0L) is isomorphic with the factor group of all cosets of the CSL in lattice 2 (in the 0-lattice). The volume of a unit cell is derived for all the lattices generated by the two crystal lattices. Secondly, the reciprocal of a lattice is introduced and the reciprocity between the CSL and the DSCL determined by the reciprocals of the two crystal lattices is shown as a special case of a theorem mentioned about modules over a ring. Finally a complete diagram of relationships between b-lattices and 0-lattices for direct lattices and reciprocal lattices is given.

Introduction

Since Bollman's 0-lattice theory (Bollmann, 1967 *a*, *b*, 1970; Bollmann & Perry 1969; Warrington & Bollmann, 1972) was derived, many theoretical studies of the coincidence-site lattice (CSL) and the complete pattern-shift lattice (DSCL) have been made. In particular, Grimmer has recently developed a general theory of the relationship between the CSL and the DSCL (Grimmer, Bollmann & Warrington, 1974; Grimmer, 1974).

In this paper we give an explicit formulation of the CSL, the DSCL, the 0-lattice and the reduced 0-lattice. We regard a lattice as a commutative group. Then the theory of groups is applicable to the lattices and in addition, the theory of numbers is another useful tool for deriving the volume of their unit cells, when one of the crystal lattices is a superlattice of the other.

Throughout this work, lattices 1 and 2 can be associated with arbitrary crystals as long as the 0-lattice and the R0L are taken into account. However, in the latter case the two crystals are related by a matrix with non-zero determinant. For simplicity we assume that the two crystal lattices are related by a non-singular matrix A, unless otherwise mentioned. All rotation matrices are naturally non-singular.

This paper is composed of two parts. Part I deals with direct lattices and Part II with reciprocals and relationships between direct lattices and their reciprocals.

PART I

1.1 The definition of a lattice and formulations of CSL, DSCL, 0-lattice and R0L

We denote in this paper:

Λ_1: lattice 1 with a basis $\{\mathbf{e}_1,\mathbf{e}_2,\mathbf{e}_3\}$

Λ_2: lattice 2 with a basis $\{\mathbf{f}_1,\mathbf{f}_2,\mathbf{f}_3\}$ such that $\mathbf{f}_i=A\mathbf{e}_i$,

where A is a non-singular matrix (having non-zero determinant)

Λ_C: CSL of Λ_1 and Λ_2

Λ_0: 0-lattice of Λ_1 and Λ_2

Λ_R: R0L of Λ_1 and Λ_2

Λ_D: DSCL of Λ_1 and Λ_2.

Each lattice Λ is the set of all integer coefficient linear combinations of its basis. Then lattice Λ can be considered to have a commutative group structure.* We also use the same notation Λ to describe this group.

Now we introduce a mathematical term 'B-module' in order to define a lattice in the most useful way: A ring B is a set, together with two laws of composition called multiplication and addition respectively, and written as a product and as a sum respectively, satisfying the following conditions:

1. With respect to addition, B is a commutative group.
2. The multiplication is associative, and has a unit element.
3. For all x,y,z in B we have $(x+y)z=x\,.\,z+y\,.\,z$ and $z(x+y)=z\,.\,x+z\,.\,y$.

* A group G is commutative, if $x.y=y.x$ for any two elements x, y in G. In this case, the notation $x+y$ is customarily used instead of $x.y$.

If B is commutative with respect to multiplication, ring B is called a commutative ring. Let B be a commutative ring. A module over B, or a B-module M is a commutative group, usually written additively, together with an operation of B on M such that, for all a, b in B and x,y in M we have $(a+b)x=ax+bx$ and $a(x+y)=ax+ay$ (Lang, 1965).

If any element of a B-module M is expressed by a unique B-coefficient linear combination of finite elements suitably chosen in M, B-module M is called finite dimensional, and the number of elements is the dimension of M. The set of the elements is a basis of M; in this case in particular, it is a finite basis.

Any commutative group is a $\mathbf{Z}$-module, where $\mathbf{Z}$ is a set of all integers; then $\mathbf{Z}$ is a commutative ring.

The following definition of a lattice is obtained:

Definition 1. A lattice is a $\mathbf{Z}$-module with a finite basis. In crystallography, the dimension of a lattice is equal to or less than 3.

We can also define a superlattice using algebraic terminology.

Definition 2. A superlattice of a lattice is a submodule† of the $\mathbf{Z}$-module associated with the lattice.

It is notable concerning definitions 1 and 2 that two lattices are identical if they are brought completely into coincidence by a translation, since every point of a lattice is identified by its position vector.

The intersection of lattices Λ_1 and Λ_2 ($\Lambda_1\cap\Lambda_2$) is always a $\mathbf{Z}$-module.‡ Then $\Lambda_1\cap\Lambda_2$ is a lattice, which is a coincidence site lattice of Λ_1 and Λ_2, written as Λ_C. The sum of lattices Λ_1 and Λ_2 ($\Lambda_1+\Lambda_2$)§ is also a $\mathbf{Z}$-module. The two newly defined lattices have the following nature.

Theorem 1. (i) Lattice Λ_C is the largest lattice contained in both Λ_1 and Λ_2. (ii) Lattice $\Lambda_1+\Lambda_2$ is the smallest lattice containing both Λ_1 and Λ_2. Let Λ and Λ' be lattices such that Λ contains Λ', *i.e.* $\Lambda\supset\Lambda'$. Λ is said to be larger than Λ' and Λ' smaller than Λ.]

Proof. (i) Let Λ_C' be a lattice contained in Λ_1 and Λ_2. Then, Λ_C' is contained in $\Lambda_C=\Lambda_1\cap\Lambda_2$. Therefore, Λ_C is the largest among the lattices contained in Λ_1 and Λ_2. (ii) Let Λ be the smallest lattice containing Λ_1 and Λ_2. Since $\Lambda_1=\Lambda_1+\{\mathbf{0}\}\subset\Lambda_1+\Lambda_2$ and $\Lambda_2=\{\mathbf{0}\}+\Lambda_2\subset\Lambda_1+\Lambda_2$, then $\Lambda_1+\Lambda_2$ is a lattice containing Λ_1 and Λ_2. Hence $\Lambda\subset\Lambda_1+\Lambda_2$.

Next, we prove that $\Lambda\supset\Lambda_1+\Lambda_2$.

$$\Lambda_1+\Lambda_2=\{\sum_i \mathrm{m}_i\mathbf{e}_i+n_i\mathbf{f}_i;\quad m_i,n_i\in\mathbf{Z}\}\,.$$

† A submodule N of a B-module is an additive subgroup such that $BN\subset N$.

‡ It is possible that the intersection of the lattices is empty. However, this disadvantage is easily removed. In fact, the intersection has at least one point which is a unit vector for the law of addition, *i.e.* a zero-vector.

§ $\Lambda_1+\Lambda_2$ is the set of vectors $\mathbf{x}_1+\mathbf{x}_2$ for all $\mathbf{x}_i$ in Λ_i.

The definition of Λ says that

$$\mathbf{e}_i \in \Lambda_1 \subset \Lambda \quad \text{and} \quad \mathbf{f}_i \in \Lambda_2 \subset \Lambda\,,$$

from which

$$\sum_i m_i\mathbf{e}_i + n_i\mathbf{f}_i \in \Lambda\,,$$

since Λ is a **Z**-module. Thus

$$\Lambda \supset \Lambda_1 + \Lambda_2$$

is proved.

If a grain boundary is nearly a coincidence boundary and a particular atomic configuration is repeated along the boundary, only certain line defects can occur in it. The line defects are called grain-boundary dislocations, the Burgers vectors of which generate a lattice, the smallest lattice containing Λ_1 and Λ_2, called the DSCL and here denoted by Λ_D. According to theorem 1, Λ_D is the lattice $\Lambda_1 + \Lambda_2$.

Lattices Λ_0 and Λ_R were first introduced by Bollmann (1967 *a*, *b*, 69). From his definition, the 0-lattice and the R0L are expressed as follows:

$$\Lambda_0 = \{\mathbf{x};\quad (I - A^{-1})\mathbf{x} \in \Lambda_1\}^*$$

where I is the unit matrix, and

$$\Lambda_{R_i} = \Lambda_0 + \Lambda_i \quad \text{for} \quad i = 1, 2\,.$$

which is the set of all position vectors generated from all translations of Λ_0 by any vector in Λ_i. The definition of Λ_0 admits that Λ_0 contains Λ_C as a superlattice. Group theory is sufficient in Part I. The notion of module plays an important role mainly in Part II.

1.2 The homomorphism of the R0L into the DSCL

We give the relationship of the R0L to the DSCL. Λ_{R_1} is taken in this section as an R0L.

Theorem 2. Λ_{R_1} is homomorphic† to a subgroup of Λ_D. The homomorphism of Λ_{R_1} into Λ_D is given by AT, where

$$T = I - A^{-1}.$$

Proof. From the definition of Λ_{R_1} we have:

$$\Lambda_{R_1} = \Lambda_0 + \sum_i \mathbf{Z}\mathbf{e}_i \qquad (1)$$

where

$$\sum_i \mathbf{Z}\mathbf{e}_i = \{\sum_i n_i\mathbf{e}_i;\quad n_i \text{ in } \mathbf{Z}\}\,.$$

Operating the linear mapping AT on equation (1), we find:

$$AT\Lambda_{R_1} = AT\Lambda_0 + \sum_i \mathbf{Z}AT\mathbf{e}_i\,.$$

Since

$$AT\Lambda_0 \subsetneqq_g A(\sum_i \mathbf{Z}\mathbf{e}_i) = \sum_i \mathbf{Z}\mathbf{f}_i‡$$

and

$$AT\mathbf{e}_i = A(I - A^{-1})\mathbf{e}_i = \mathbf{f}_i - \mathbf{e}_i\,,$$

then

$$AT\Lambda_{R_1} \subsetneqq_g \sum_i (\mathbf{Z}\mathbf{e}_i + \mathbf{Z}\mathbf{f}_i) = \Lambda_D\,.$$

Following Bollmann's (1970) notation, the DSCL is lattice $\Lambda^{(2-sc)}$ of all $d^{(2-sc)}$ vectors. All the translations of $d^{(2-sc)}$ keep a periodic-pattern configuration unchanged. According to the theorem, a translation of the primary 0-point, which is a coincidence site, involves a translation of lattice 2, $\sum_i m_i\mathbf{e}_i + n_i\mathbf{f}_i$, to conserve the elements of the pattern.

1.3 Volumes of unit cells for the DSCL and the R0L

The following theorems establish a more concrete comparison between the DSCL and the R0L. In this section we assume that matrix A is unimodular, that is, the determinant of A is 1 or -1. A homomorphism of a group G into another G', is called an isomorphism if the homomorphism is bijective, *i.e.* one-to-one. In this case, we say that G is isomorphic to G' and we can identify G with G' as a group. The existence of an isomorphism between G and G' is denoted by $G \cong G'$.

If G_1 is a normal subgroup§ of group G, the set of all cosets of G_1 in G is a group which is called the factor group of G and denoted by G/G_1. Any subgroup of a commutative group is normal. Then a factor group is always possible to be made with a lattice and its superlattice.

Theorem 3

(i) $\Lambda_D/\Lambda_1 \cong \Lambda_2/\Lambda_C$

(ii) $\Lambda_{R_1}/\Lambda_1 \cong \Lambda_0/\Lambda_C$

Proof. (i) From the isomorphism theorem‖ well known in group theory, the factor group $\Lambda_D/\Lambda_1 = (\Lambda_1 + \Lambda_2)/\Lambda_1$ is isomorphic to $\Lambda_2/\Lambda_1 \cap \Lambda_2$, from which

$$\Lambda_D/\Lambda_1 \cong \Lambda_2/\Lambda_C\,.$$

(ii) Similarly,

$$\Lambda_{R_1}/\Lambda_1 = (\Lambda_0 + \Lambda_1)/\Lambda_1 \cong \Lambda_0/\Lambda_1 \cap \Lambda_0\,.$$

* Bollmann (1970) defined the 0-lattice as a set of $\mathbf{x}$ such that $(I - A^{-1})\mathbf{x} \in \Lambda_1$ and $(I - A^{-1})\mathbf{x} \neq \mathbf{0}$.
He excluded trivial 0-points (*e.g.* points on an axis of rotation). In this paper, Λ_0 is defined without the condition $(I - A^{-1})\mathbf{x} \neq \mathbf{0}$. Therefore, Λ_C is always contained in Λ_0 even if the determinant of matrix $(I - A^{-1})$ is zero.

Furthermore, Λ_0 is a **Z**-module.

In fact, $T = I - A^{-1}$ is a homomorphism. The inverse image of a B-module is a B-module if a mapping is a homomorphism. Λ_0 is the inverse image of homomorphism T of a sub-module of **Z**-module Λ_1; *i.e.* Λ_1 itself, a lattice plane of Λ_1, a lattice line of Λ_1 or a lattice point $\{\mathbf{0}\}$ of Λ_1 according to rank $(T) = 3, 2, 1$ or 0.

† A homomorphism, f, of a group G into another G' is a mapping such that $f(x\,.\,y) = f(x)\,.\,f(y)$ for all x, y in G, in the case where G is called homomorphic to G' (under a homomorphism f).

‡ Subgroup G_2 of group G_1 is denoted by $G_2 \subsetneqq_g G_1$.

§ Subgroup G_1 is normal, when $xG_1 = G_1x$ for all elements x in G.

‖ p. 18 in Lang (1965) or Theorem 2·4·1 in Hall (1959).

Let $\mathbf{x}$ be an element of $\Lambda_C=\Lambda_1\cap\Lambda_2$. Then,

$$T\mathbf{x}=\mathbf{x}-A^{-1}\mathbf{x}\in\Lambda_1 .$$

Hence $\mathbf{x}\in\Lambda_0$ and $\mathbf{x}\in\Lambda_1\cap\Lambda_0$.
Conversely, let $\mathbf{x}'$ be an element of $\Lambda_1\cap\Lambda_0$. Then,

$$\mathbf{x}'-A^{-1}\mathbf{x}'\in\Lambda_1 ,$$

from which

$$A^{-1}\mathbf{x}'\in\Lambda_1 \quad \text{and so} \quad \mathbf{x}'\in A\Lambda_1=\Lambda_2 .$$

Therefore, we see that $\Lambda_C=\Lambda_1\cap\Lambda_0$. Then

$$\Lambda_{R_1}/\Lambda_1\cong\Lambda_0/\Lambda_C .$$

As a corollary we take the following:

Corollary

$$\Lambda_C=\Lambda_1\cap\Lambda_0=\Lambda_2\cap\Lambda_0 .$$

Proof. The first equality has been shown in the proof of theorem 3. Here, the proof will be given for the other. From $\Lambda_C=\Lambda_1\cap\Lambda_2=\Lambda_1\cap\Lambda_0$, we find:

$$\Lambda_C\subset\Lambda_2 \quad \text{and} \quad \Lambda_C\subset\Lambda_0 .$$

Then $\Lambda_C\subset\Lambda_2\cap\Lambda_0$.
Conversely, if we take any $\mathbf{x}$ in $\Lambda_2\cap\Lambda_0$, then

$$\mathbf{x}-A^{-1}\mathbf{x}\in\Lambda_1 \quad \text{and} \quad \mathbf{x}\in\Lambda_2 .$$

From $\mathbf{x}\in\Lambda_2$
we obtain $A^{-1}\mathbf{x}\in\Lambda_1$.
Thus $\mathbf{x}=(\mathbf{x}-A^{-1}\mathbf{x})+A^{-1}\mathbf{x}\in\Lambda_1$.
The corollary is therefore proved.

Theorem 3 says that factor group Λ_D/Λ_1 (or Λ_{R_1}/Λ_1) is identical with factor group Λ_2/Λ_C (or Λ_0/Λ_C) which is composed of all cosets of Λ_C in Λ_2 (or Λ_0). Λ_D/Λ_1 is expressed by all the representatives of cosets or equivalence classes (Bollmann, 1970) of Λ_D in the unit cell of lattice 1. This will also be so for Λ_{R_1}/Λ_1.

Let Λ_α be a lattice, Λ_β a superlattice (or sublattice) of Λ_α and V_α, V_β the volumes of their corresponding unit cells. We denote the number of elements in a group G by ord (G).

Theorem 4

$$V_\beta/V_\alpha=\text{ord}\ (\Lambda_\alpha/\Lambda_\beta)$$

where $\Lambda_\alpha/\Lambda_\beta$ is the factor group of all cosets of Λ_β.
Proof. From a theorem in the theory of numbers (Takagi, 1958), the volume of a parallelepiped built up with lattice sites at its vertices is equal to the number of lattice sites in it.* Then we find that the volume of the unit cell of superlattice Λ_β is a multiple of V_α and the number of lattice sites of Λ_α in the unit cell of Λ_β. The lattice sites in the unit cell of Λ_β can be taken as representatives of all cosets in factor group $\Lambda_\alpha/\Lambda_\beta$. We therefore see that the theorem holds.

* Special attention must be paid to the expression 'in it'. It means that lattice sites on the faces are counted once for a pair of opposite faces, ones on the segments once for a set of four parallel edges and ones at the vertices once for a set of all the eight vertices.

Values Σ and σ are defined respectively as a ratio V_C to V_1 and a ratio V_C to V_0.

Proposition 1. $V_0=(\Sigma/\sigma)V_1$.

Theorem 4 says that

$$\Sigma=\text{ord}\ (\Lambda_1/\Lambda_C) \quad \text{and} \quad \sigma=\text{ord}(\Lambda_0/\Lambda_C) .$$

Therefore, Σ and σ are positive integers equal to or greater than 1.† If $\Lambda_1=\Lambda_2$, then $\Lambda_C=\Lambda_1$ and $\Sigma=1$. Conversely, if $\Sigma=1$, then $\Lambda_1=\Lambda_2$. Therefore,

Proposition 2. $\Sigma=1$ is equivalent to $\Lambda_1=\Lambda_2$.

Σ and σ values have other equivalent definitions, such as: Σ is the reciprocal of the density of common sites (Brandon, Ralph, Ranganathan & Wald, 1964) and σ is the number of lattice sites of Λ_0 in the unit cell of Λ_C, namely the number of distinct pattern elements. The equivalence of the definitions can be easily seen from theorem 3.

As a direct consequence of theorems 3 and 4, theorem 5 is derived.

Theorem 5

$$V_D=(1/\Sigma)V_1$$

$$V_{R_1}=(1/\sigma)V_1 .$$

In the case of $\langle 100\rangle$ 22·61° rotation with $\Sigma=13$ for cubic crystals, σ is equal to 2. Then the volume of a unit cell for the DSCL is about six times smaller than that for the R0L.

From theorem 5 and the definition of σ, we obtain:

Proposition 3 $\sigma=1$ is equivalent to $\Lambda_0=\Lambda_C$, $\Lambda_0\subset\Lambda_1$ or $\Lambda_{R_1}=\Lambda_1$.

According to proposition 3, $\sigma=1$ means that there is an equivalence class of 0-points, *i.e.* an equivalence class of zero-vectors.

Theorem 6 is then obtained.

Theorem 6

(i) $\Sigma:=V_C/V_1=V_1/V_D=V_0/V_{R_1}$‡§

(ii) $\sigma:=V_C/V_0=V_1/V_{R_1}$.

It is notable in theorem 6 that the ratio V_0/V_{R_1} is also equal to Σ, the corresponding lattices of which belong to the category of 0-lattices.

1.4 Transcendental lattice

We introduce a lattice generated by crystal lattices Λ_1 and Λ_2 and 0-lattice Λ_0. The lattice is called the transcendental lattice and denoted by Λ_t. The proof of the following propositions is given in the Appendix.

† If Λ_C or Λ_0 is a set consisting of one element, *i.e.* a zero vector, Σ or σ is defined as infinity.

‡ The symbol: = means equality by definition (Grimmer *et al.*, 1974).

§ $\Sigma=V_0/V_{R_1}$ is proved by $\Lambda_1/\Lambda_C=\Lambda_1/\Lambda_1\cap\Lambda_0\cong(\Lambda_1+\Lambda_0)/\Lambda_0=\Lambda_{R_1}/\Lambda_0$.

Proposition 4

(i) $\Lambda_t := \Lambda_1 + \Lambda_2 + \Lambda_0 = \Lambda_D + \Lambda_0 = \Lambda_1 + \Lambda_{R_2} = \Lambda_2 + \Lambda_{R_1}$

(ii) $\Lambda_C = \Lambda_D \cap \Lambda_0 = \Lambda_1 \cap \Lambda_{R_2} = \Lambda_2 \cap \Lambda_{R_1}$.

Proposition 5

(i) $\Lambda_t/\Lambda_D \cong \Lambda_{R_i}/\Lambda_i$ or $\Lambda_t/\Lambda_{R_i} \cong \Lambda_D/\Lambda_i$ $(i=1,2)$

(ii) $\Lambda_t/\Lambda_{R_1} \cong \Lambda_{R_2}/\Lambda_0$

(iii) $\Lambda_t/\Lambda_0 \cong \Lambda_D/\Lambda_C$

(iv) $\Lambda_t/\Lambda_{R_2} \cong \Lambda_1/\Lambda_C$, $\Lambda_t/\Lambda_{R_1} \cong \Lambda_2/\Lambda_C$.

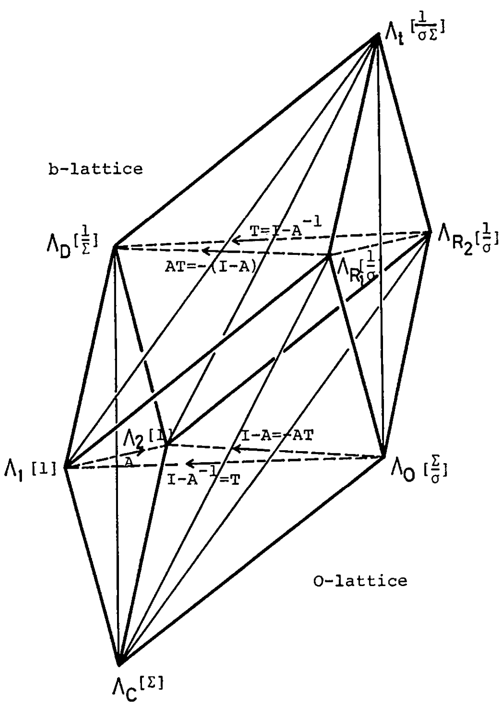
The volume of a unit cell of the transcendental lattice, V_t, is found from one of the relations in proposition 5.

Proposition 6

$$V_t = (1/\sigma\Sigma)V_1 .$$

The transcendental lattice is the coarsest lattice that contains not only lattices Λ_1 and Λ_2 but also Λ_0 and Λ_D as superlattices.

From the theorems and propositions, we conclude the relationship of superlattice and the relationships between the DSCL and the CSL depicted in Fig. 1. For lattices joined by a segment the lower is a superlattice of the upper. For every parallelogram a lattice related to lattices Λ and Λ' by segments in lower or upper position on the parallelogram is respectively the CSL or DSCL of lattices Λ and Λ'. The value associated with each lattice in brackets is the volume of its unit cell if $V_1=1$. The homomorphism between lattices is given with an arrow to express the homomorphism relationship.



(Direct lattices)

Fig. 1. The explicit representation of relationships between b-lattices and 0-lattices. The parallelepiped consists of the parallelograms of the CSL and DSCL of two lattices situated at the medium vertices of each parallelogram.

PART II

2.1 Introduction to part II

We have introduced a mathematical term 'B-module' in §1.1. The reciprocal of a B-module is defined, which leads to the specification of a reciprocal lattice. The CSL, 0-lattice, R0L and DSCL are defined for two reciprocal lattices in the same way as for direct lattices. We prove a reciprocity between the CSL of direct lattices and the DSCL of their reciprocal lattices.†

2.2 Definition of reciprocal lattice

Let M be a module over a commutative ring B and admit a finite basis, say $\{e_1, e_2, \ldots, e_m\}$. A reciprocal module of M is defined as a B-module with a basis $\{f_1, f_2, \ldots, f_m\}$ which is the functional‡ such that

$$f_i(e_j) = \delta_{ij}$$

or written as $\langle e_j, f_i \rangle = \delta_{ij}$ with Kronecker's delta δ_{ij}. The reciprocal of M is denoted by M^*.

2.3 Reciprocity between the CSL of direct lattices and the DSCL of their reciprocal lattices

We introduce several theorems without proof (see Lang, 1965).

Theorem 1

$$M \cong M^* ,$$

that is, a B-module is isomorphic to its reciprocal. As a corollary of theorem 1, we get:

Corollary

$$M \cong M^{**} .$$

Under this isomorphism, M is usually identified with M^{**}. This identification and the reciprocity in theorem 1 assert that once we prove a proposition in terms of M and M^*, the proposition obtained with the interchange of M and M^* is also true.

Theorem 2. Let M_1 and M_2 be submodules of M such that

$$M_1 \subset M_2 .$$

Then

$$M_1^* \supset M_2^* .$$

In fact, any functional in M_2^* is defined on M_2. If we restrict to M_1 the domain of the functional, it is a functional defined on M_1. Therefore, we show that $M_1^* \supset M_2^*$ if $M_1 \subset M_2$.

† Grimmer (1974) has given another proof.

‡ A functional is a linear mapping of M into B.

Let M_D^* and M_C^* be the DSCL and the CSL of the reciprocals M_1^* and M_2^*. That is:

$$M_D^* = M_1^* + M_2^* \quad \text{and} \quad M_C^* = M_1^* \cap M_2^* .$$

The reciprocals of M_D and M_C are denoted by $(M_D)^*$ and $(M_C)^*$. We shall prove the theorem of reciprocity.

Theorem 3 (*Theorem of reciprocity*)

$$M_D^* = (M_C)^*, \quad (M_D)^* = M_C^*$$

Proof. When M_1 and M_2 are replaced respectively by M_1^* and M_2^*, the former is equivalent to the latter. We shall prove that $M_D^* = (M_C)^*$.

First, it will be shown that $M_D^* \subset (M_C)^*$.
From the definition of M_C,

$$M_C \subset M_i , \quad \text{then } (M_C)^* \supset M_i^* \quad \text{for } i=1,2.$$

Since reciprocal M_D^* is the smallest module containing M_1^* and M_2^*,

$$M_D^* \subset (M_C)^*$$

is proved.

Secondly, we shall see that $(M_C)^* \subset M_D^*$.
Since

$$M_i^* \subset M_D^*,$$

$$M_i = M_i^{**} \supset (M_D^*)^* \quad \text{for } i=1,2$$

and

$$M_C \supset (M_D^*)^*.$$

Therefore

$$(M_C)^* \subset M_D^* .$$

Consequently we have shown that

$$M_D^* = (M_C)^*.$$

As a special case of B-modules, a reciprocity relationship for lattices is obtained:

Theorem of reciprocity for lattices

$$\Lambda_D^* = (\Lambda_C)^* \quad \text{or} \quad (\Lambda_D)^* = \Lambda_C^* ,$$

Theorem 4 admits that $\Lambda_D^* = (\Lambda_C)^*$ or $(\Lambda_D)^* = \Lambda_C^*$ is true for arbitrary lattices.

Let Λ_0^* be a lattice such that

$$\Lambda_0^* = \{\mathbf{x}'; \ (I - {}^tA^{-1})\mathbf{x}' \in \Lambda_2^*\} .$$

Λ_0^* is defined as a 0-lattice in the reciprocal lattice corresponding to the 0-lattice in the direct lattice. A parallelepiped is constructed in the category of the reciprocal lattices based on lattices Λ_1^*, Λ_2^* and Λ_0^* in the same way as the parallelepiped on Λ_1, Λ_2 and Λ_0. Another parallelepiped is obtained for the reciprocals of the direct lattices schematized in Fig. 1. Coincidence vertices of the two parallelepipeds in Fig. 2 show the reciprocity relationships described in the theorem.

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APPENDIX

The proof of propositions 4 and 5 is given here.

Proof of proposition 4

(i) It is easily shown.

(ii) $\Lambda_D \cap \Lambda_0 = (\Lambda_1 + \Lambda_2) \cap \Lambda_0 = \Lambda_1 \cap \Lambda_0 + \Lambda_2 \cap \Lambda_0$
$= \Lambda_C + \Lambda_C = \Lambda_C$
$\Lambda_1 \cap \Lambda_{R_2} = \Lambda_1 \cap (\Lambda_0 + \Lambda_2) = \Lambda_1 \cap \Lambda_0 + \Lambda_1 \cap \Lambda_2 = \Lambda_C .$

Similarly,

$$\Lambda_2 \cap \Lambda_{R_1} = \Lambda_C .$$

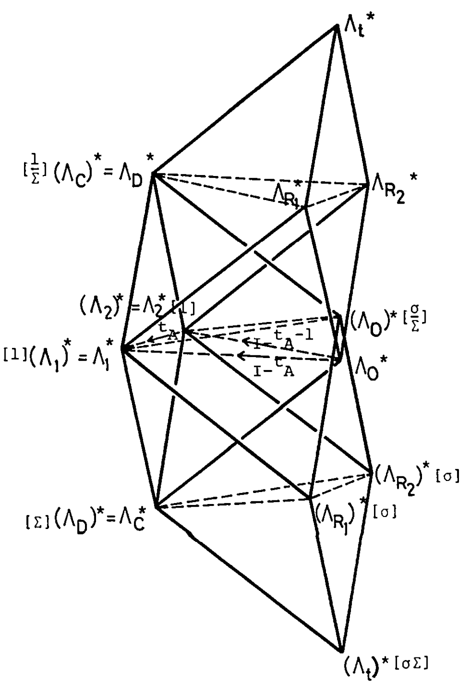
Proof of proposition 5

The theorem of isomorphism and proposition 4 asserts (iii) and (iv). To prove (i) it is sufficient to show that

$$\Lambda_t = \Lambda_D + \Lambda_{R_i} \quad \text{and} \quad \Lambda_i = \Lambda_D \cap \Lambda_{R_i} .$$

$$\Lambda_t = (\Lambda_1 + \Lambda_2) + (\Lambda_i + \Lambda_0) = \Lambda_D + \Lambda_{R_i} .$$

$$\Lambda_D \cap \Lambda_{R_i} = (\Lambda_1 + \Lambda_2) \cap (\Lambda_i + \Lambda_0) = (\Lambda_1 \cap \Lambda_i + \Lambda_2 \cap \Lambda_i) + \Lambda_1 \cap \Lambda_0 + \Lambda_2 \cap \Lambda_0 = \Lambda_i + \Lambda_C + \Lambda_C = \Lambda_i .$$



(Reciprocal lattices)

Fig. 2. Parallelepipeds constructed on Λ_1^*, Λ_2^* and Λ_0^*, and on the reciprocals of Λ_1, Λ_2 and Λ_0. Coincidence vertices of the two parallelepipeds correspond to the lattices in the reciprocity relationship. Λ_i^* and $(\Lambda_i)^*$ are the same lattices defined as the reciprocals of Λ_i $(i=1,2)$. The associated value stands for the volume of a unit cell of each lattice.

Proposition 5 (ii) is deduced from

$$A_t = A_{R_1} + A_{R_2} \quad \text{and} \quad A_0 = A_{R_1} \cap A_{R_2},$$

which are verified as for (i).

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Univalent (Monodentate) Substitution on Convex Polyhedra. II. Listing of Cycle Indices

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To extend the usefulness of the tabulation of the numbers N of positional isomers [Knop, Barker & White (1975). *Acta Cryst.* A**31**, 461–472], all the distinct cycle-index polynomials Z on which the tabulation is based have been listed in a convenient form. This condensed summary facilitates identification of Z-isomorphisms; in turn, N for univalent substitution on many polyhedra not listed previously can be evaluated simply by reference to the existing tabulation.

In part I (Knop, Barker & White, 1975) we presented the numbers N of distinct (up to rotation) positional isomers obtained by univalent substitution at the vertices of convex polyhedra; only structureless substituents were considered. The tabulation is extensive, but naturally it cannot include *all* non-isomorphic polyhedra even for small numbers of vertices V. A user of the tables wishing to evaluate N for polyhedra not listed in Table 5 of part I would not only have to determine the appropriate cycle indices Z, but he would have to compute the coefficients of the expanded cycle-index polynomials (*i.e.* the values of N) for the compositions of interest, a tedious task. However, owing to cycle-index isomorphism the number of distinct Z polynomials involved in the tabulations of part I is not unduly large, and there is a good chance that the set of N to be determined already appears there under a different but Z-isomorphic polyhedron, which makes fresh computation unnecessary.

To facilitate identification of additional Z-isomorphisms, over and above those *specifically* listed in part I, a table of *all* the cycle indices on which the tabulation of part I is based, has been compiled.

Considerable space is saved by introducing the following notation. An s-product $s_a^u s_b^v$ will be represented as $a,u*b,v$. Each s-product occurring in the cycle indices for a particular value of V will be denoted by a capital letter (Table 1). The highest-order term s_1^V (represented by A) is always present,† and so further space is saved by omitting A from the letter symbol of Z. For example, the Z of a tetrahedron **4–2** of symmetry T_d,

$$\tfrac{1}{24}(s_1^4 + 6s_4^1 + 8s_1^1s_3^1 + 6s_1^2s_2^1 + 3s_2^2),$$

is represented by $6B8C6D3E$. The s-products denoted by the letters are found in Table 1 under $V=4$. The sum of the coefficients associated with the letters, including the coefficient of A, which is always unity, is equal to the divisor $p(\mathbf{G})$, in this case 24.

For economy of space, the table of cycle indices (Table 2) is arranged as follows. In the first part (pp. 3–9) Z polynomials occurring in only a few cases are listed in the order of increasing V. The second part (pp. 9–16) contains cycle indices having large numbers of terms and those involved in considerable numbers of Z-isomorphic representations.

† The term A by itself represents $Z(4mh)$ of the corresponding polygon of V vertices (*cf.* part I).

‡ Table 2 has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 31246 (16 pp., 1 microfiche). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.