$$u_{CH}=\frac{\int W(x)\alpha_S(2u_H-2x)\mathrm{d}x}{\int W(x)\,\dfrac{\alpha_S(2u_H-2x)}{u_H-x}\,\mathrm{d}x} \tag{A8}$$

$$u_{CL}=\frac{\int W(x)\alpha_S(2u_L+2x)\mathrm{d}x}{\int W(x)\,\dfrac{\alpha_S(2u_L+2x)\,\mathrm{d}x}{u_L+x}} \tag{A9}$$

The explicit arguments of the α's are Ω values; the other parameters are understood.

Since the α's may not be known, our approximation is to replace them with the spherically averaged values. The term in braces in (A7) may then be obtained as the difference between the appropriate curve and its asymptote in Fig. 2(*b*), or analytically from (A3) and (A4). The terms in (A8) and (A9) may be read from Fig. 2(*a*) or evaluated from (A5), (A2), or (6). Surprisingly, the needed quantities may be obtained with sufficient accuracy from the Figure, but the process is somewhat tedious.

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Algorithm for Determining the Symmetry and Stacking Properties of the Planes (*hkl*) in a Bravais Lattice

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An algorithm is presented which enables one to determine in detail the symmetry and stacking properties of the planes (*hkl*) in an arbitrary Bravais lattice characterized by the quantities a, b, c, $\cos\alpha$, $\cos\beta$, $\cos\gamma$.

1. Introduction

The problem of mapping a lattice plane was originally formulated and solved by Jaswon & Dove (1955) and more recently, using the tensor formalism, by Bevis (1969). Nevertheless we believe that it is worth considering the present procedure since it possesses some new and useful features.

Firstly, all considerations refer to the *symmetry* of the plane (*hkl*) which was discussed neither by Jaswon & Dove nor by Bevis.

Secondly, our results, unlike those of the above authors, are presented in a unique way. This is, of course, important when comparing various calculations and compiling tables. The following example shows it clearly. Jaswon & Dove determine in their paper the configuration of the lattice points in the plane (295) in a primitive cubic lattice to be a parallelogram of edges $\sqrt{29}$ and $\sqrt{106}$ and included angle $\cos^{-1}18/(\sqrt{29\times 106})$. This parallelogram contains four interior lattice points in addition to those at its corners. If they applied their procedure to the equivalent planes (952) and (259) they would have obtained quite different parallelograms with 1 and 8 interior lattice points, respectively. Alternatively the tables obtained from our algorithm give the cell of edges $\sqrt{19}$ and $\sqrt{6}$ and included the angle $\cos^{-1}(\sqrt{114}/57)$. These numbers are unique, since the cell is primitive and has the shortest possible perimeter. Also the symmetry of the plane can be readily recognized. Moreover it is not immediately patent that the results by Jaswon & Dove and ourselves are identical.

Similar comment applies to the procedureof Bevis. Though the resulting parallelogram here is without interior points, its shape depends on the choice of the integers m_1, m_2, m_3 satisfying the Diophantine equation

$$m_1u^1+m_2u^2+m_3u^3=1\ .$$

But this equation has infinitely many solutions provided the u^i are integers without common factor.

Thirdly our procedure is formulated as an algorithm and this way has some advantages, too. The greatest, of course, is the possibility of applying a computer directly. Further the process can be phrased as short as possible since all auxiliary concepts may be adjourned to the proof, which may be easily performed in a rigorous way customary in contemporary mathematics. According to our opinion the root of the problem lies much more in the theory of numbers than in geometry and therefore tensor formalism has not been used.

The original theses, of which the present paper is an abridgement, involve a full discussion of the concepts *mesh* and *fundamental cell*, especially the proofs of their uniqueness which motivates the convenience of them. It turned out that although these concepts are very intuitive ones the rigorous proofs are not simple at all. Although this discussion has not been included in the present paper for the sake of brevity, we considered it useful to quote the definitions of these concepts and give the theorems concerning their uniqueness at least without proofs. The achievement of rigorous and pure formulations, concepts and proofs was one of our chief aims.

Two-dimensional Bravais lattices may be divided according to their symmetry into 5 classes, namely those consisting of squares, rectangles, equilateral triangles, rhombs or only rhomboids. In the present paper we are interested in the symmetry and stacking properties of two-dimensional lattices lying in the rational planes (hkl) of a three-dimensional Bravais lattice. The relationship between this lattice and its two-dimensional parts need not be particularly simple. For example, in the primitive orthorhombic lattice ($\cos\alpha=\cos\beta=\cos\gamma=0$) the planes (123) consist of squares if $6a^2=3b^2=2c^2$, of equilateral triangles if $24a^2=3b^2=8c^2$, of rectangles if either $6a^2=3b^2\neq 2c^2$ or $a^2-2b^2-c^2=0$, of rhombs in the following six cases: $24a^2=3b^2\neq 8c^2$, $8(b^2-5a^2)=8c^2\neq 3b^2$, $3b^2\neq 24a^2=8c^2\neq 12b^2$, $3a^2-3b^2-c^2=0$, $a^2-5b^2-3c^2=0$, $a^2-8b^2-3c^2=0$; and in all other cases only of rhomboids. The knowledge of the symmetry and stacking properties of rational planes may be useful in various problems. We need only mention stacking faults and twins with rational composition planes. Some other applications are mentioned in the papers listed at the end.

Our results are formulated in two theorems, referring respectively to the symmetry and stacking of lattice planes, and one algorithm. The reasons for this division are not only formal. The algorithm shows a certain way how to find the integral numbers needed in the theorems; in special cases, *e.g.* solving other similar problems, it may be possible to find them in a shorter way and to use the theorems directly.

The algorithm is phrased in such a manner that a computer can be immediately applied. Two procedures in ALGOL 60 were developed by the author.* One of them, using *real* quantities, is applicable to any Bravais lattice and any rational plane. The other relates to 10 of the 14 types of Bravais lattices (namely those with $\cos\alpha=\cos\beta=\cos\gamma=0$ and the hexagonal) provided that a, b, c are integers. Here only *integer* quantities are used and the decision about the shape of the two-dimensional lattice may be done by the computer itself. By means of these procedures tables for primitive, face-centred and body-centred cubic lattices involving planes (hkl) up to Max $(|h|,|k|,|l|)=10$ were calculated.*

It may be perhaps of some interest that the algorithm is applicable not only when the lattice and the plane are given numerically. Also general discussions are possible when the shape of the lattice depends on one or two (or perhaps more) parameters (see the above example). A preliminary account of the algorithm was presented by Gruber (1966).

2. Notation and auxiliary concepts

The five shapes of parallelograms are denoted as follows: **S** – square; **R** – rectangle (which is not an **S**); **E** – rhomb with two 60° angles; **D** – rhomb (which is neither **S** nor **E**); **P** – rhomboid (which is neither of **S**, **R**, **E**, **D**). The symbol $[a]$ (a a real number) will be used, as usual, for the integer satisfying $0\le a-[a]<1$. The symbol HCF $(h_1,\ldots,h_n)$ ($h_1,\ldots,h_n$ integers not all equal to zero) designates the positive highest common factor of the numbers $h_1,\ldots,h_n$. The meaning of the expressions $\mathbf{t}=B-A$, $B=A+\mathbf{t}$ (A, B points, $\mathbf{t}$ vector) is clear. If $\mathbf{a},\mathbf{b},\mathbf{c}$ are linearly independent lattice vectors of a Bravais lattice M, then $[\mathbf{a},\mathbf{b},\mathbf{c}]_M$ designates the set of all unit cells U of M possessing this property: there exist such corners O,A,B,C of the cell U that $\mathbf{a}=A-O$, $\mathbf{b}=B-O$, $\mathbf{c}=C-O$. Similarly we define the symbol $[\mathbf{a},\mathbf{b}]_N$ for a two-dimensional lattice N.

Consider now a two-dimensional Bravais lattice N. Any of its unit cells with shortest perimeter will be referred to as a *fundamental cell*. Such a cell is always primitive. A unit cell U of the lattice N is termed its *mesh*, if it represents the symmetry properties of this lattice. Rigorously, if it is primitive and one of these two cases occurs: (1) U is not a **P**; (2) U is a **P**, U is a fundamental cell of N and all primitive unit cells of N are **P**'s. For these two concepts simple assertions are valid: *Any two fundamental cells of the lattice N are congruent. Any two meshes of the lattice N are congruent.* Thus denoting by p, q ($p\le q$) the lengths of the sides and by ψ ($\psi\le 90°$) the size of the angle of a fundamental cell of N, these quantities are uniquely determined by N. The same may be said about the quantities x,y,φ introduced in a similar way for a mesh of N. The mutual relationship is shown in Table 1.

Accordingly a fundamental cell is simultaneously a mesh unless $2pq\cos\psi=p^2<q^2$.

Further let N' be another two-dimensional Bravais lattice which has originated from N by translation. This translation is determined by any vector $\mathbf{r}$ connecting a point of N with a point of N'. For our purposes it is convenient to relate this vector either to a fundamental cell or to a mesh of N. Real numbers

* They may be obtained from the author on request.

$$t_1, t_2, t_3 \tag{1}$$

(in this order) will be referred to as *parameters of the mutual displacement* (p.m.d.) of the lattices N, N' with respect to fundamental cells, if points $O \in N$, $O' \in N'$ and vectors $\mathbf{p}, \mathbf{q}, \mathbf{k}$ exist in such a way that

(1) $[\mathbf{p}, \mathbf{q}]_N$ are fundamental cells of N;
(2) $|\mathbf{p}| \le |\mathbf{q}|$, $\mathbf{p} \cdot \mathbf{q} \ge 0$;
(3) $|\mathbf{k}| = 1$, $\mathbf{p} \cdot \mathbf{k} = \mathbf{q} \cdot \mathbf{k} = 0$;
(4) $t_1\mathbf{p} + t_2\mathbf{q} + t_3\mathbf{k} = O' - O$.

If p.m.d. (1) fulfil $0 \le t_1 < 1$, $0 \le t_2 < 1$, $t_3 \ge 0$, they are said to be *standard*. In a similar way we define the p.m.d.

$$t'_1, t'_2, t'_3 \tag{2}$$

of the lattices N, N' with respect to meshes.

The standard p.m.d. are not uniquely determined by the lattices N and N', nor is the lattice N' uniquely determined by the lattice N and the p.m.d. But this gives no trouble. The significance of these concepts may be seen from the following assertion: *If N' and N'' have originated from N by translation and if* (1) *are p.m.d. of N, N' as well as of N, N'', then the sets $N \cup N'$, $N \cup N''$ are congruent*. This means that the lattices N, N' have the same 'relative position' as the lattices N, N''; and we are only interested in this relative position.

Therefore, by p.m.d. of the planes $(h\,k\,l)$ (with respect to fundamental cells or to meshes) we understand the p.m.d. of the lattices N, N' lying in two neighbouring $(h\,k\,l)$ planes.

3. Theorems and algorithm

In this paragraph a three-dimensional Bravais lattice M and rational planes $(h\,k\,l)$ are given. The integers h,k,l relate to a primitive unit cell U of M characterized by the quantities a, b, c, $\cos\alpha$, $\cos\beta$, $\cos\gamma$. Thus denoting

$$X = 1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma\,,$$

the inequality $X > 0$ is satisfied. The assumption that U is primitive is essential as well as the fact that h,k,l are without common factor. A two-dimensional lattice N lying in one of the planes $(h\,k\,l)$ is chosen,

$$p, q, \psi\,, \quad x, y, \varphi \tag{3}$$

having the same meaning (with respect to N) as in § 2. The following notation is applied throughout:

$$\begin{aligned}
V &= H^2a^2 + K^2b^2 + L^2c^2 + 2HKab\cos\gamma \\
&\quad + 2HLac\cos\beta + 2KLbc\cos\alpha \\
V' &= H'^2a^2 + K'^2b^2 + L'^2c^2 + 2H'K'ab\cos\gamma \\
&\quad + 2H'L'ac\cos\beta + 2K'L'bc\cos\alpha \\
W &= HH'a^2 + KK'b^2 + LL'c^2 + (HK' + KH')\,ab\cos\gamma \\
&\quad + (HL' + LH')ac\cos\beta + (KL' + LK')bc\cos\alpha \\
U &= HH^*a^2 + KK^*b^2 + LL^*c^2 + (HK^* \\
&\quad + KH^*)ab\cos\gamma + (HL^* + LH^*)ac\cos\beta \\
&\quad + (KL^* + LK^*)bc\cos\alpha \\
U' &= H'H^*a^2 + K'K^*b^2 + L'L^*c^2 + (H'K^* \\
&\quad + K'H^*)ab\cos\gamma + (H'L^* + L'H^*)ac\cos\beta \\
&\quad + (K'L^* + L'K^*)bc\cos\alpha \\
Y &= VV' - W^2
\end{aligned} \tag{4}$$

$$\begin{aligned}
&T_1 = (UV' - U'W)/Y \qquad T_2 = (U'V - UW)/Y \\
&t_1 = T_1 - [T_1] \qquad\qquad\quad t_2 = T_2 - [T_2] \\
&t'_1 = \begin{cases} -t_1 - [-t_1] \ldots\ldots & \text{if } 2W = V < V' \\ t_1 \ldots\ldots\ldots\ldots\ldots & \text{in other cases} \end{cases} \\
&t'_2 = \begin{cases} t_1 + t_2 - [t_1 + t_2] \ldots & \text{if } 2W = V < V' \\ t_2 \ldots\ldots\ldots\ldots\ldots & \text{in other cases} \end{cases} \\
&t'_3 = t_3 = abc\sqrt{X}/Y\,,
\end{aligned} \tag{5}$$

Table 1. *Relationship between fundamental cell and mesh*

Fundamental cell							Mesh			
0		$2pq\cos\psi$		p^2		q^2	Shape	x	y	$\cos\varphi$
	=				=		**S**	p		
	=				<		**R**	p	q	
			=		=		**E**		q	
			=		<		**D**		q	$1 - 2\cos^2\psi$
	<		<		=		**D**		q	$\cos\psi$
	<		<		<		**P**	p	q	$\cos\psi$

Table 2. *Determination of the shape and size of meshes*

Conditions							Mesh			
0		$2\|W\|$		V		V'	Shape	x	y	$\cos\varphi$
	=				=		**S**	$\sqrt{V}$		
	=				<		**R**	$\sqrt{V}$	$\sqrt{V'}$	
			=		=		**E**		$\sqrt{V'}$	
			=		<		**D**		$\sqrt{V'}$	$1 - V/2V'$
	<		<		=		**D**		$\sqrt{V'}$	$\|W\|/V'$
	<		<		<		**P**	$\sqrt{V}$	$\sqrt{V'}$	$\|W\|/\sqrt{VV'}$

the meaning of $H, H', H^*, \ldots$ being made clear in the theorems.

Theorem 1

Let the integers

$$H, K, L, \quad H', K', L' \qquad (6)$$

fulfil

$$hH+kK+lL=0\,, \quad hH'+kK'+lL'=0\,, \qquad (7)$$

$$\mathrm{HCF}\left(\begin{vmatrix} H & K \\ H' & K' \end{vmatrix}, \begin{vmatrix} H & L \\ H' & L' \end{vmatrix}, \begin{vmatrix} K & L \\ K' & L' \end{vmatrix}\right)=1\,, \qquad (8)$$

$$2|W| \le V \le V' \qquad (9)$$

(such integers (6) do always exist). Then

$$p=\sqrt{V}\,, \quad q=\sqrt{V'}\,, \quad \cos\psi=|W|/\sqrt{VV'} \qquad (10)$$

holds for the fundamental cells of N and the shape and size of the meshes of N can be read off the Table 2.

Theorem 2

Let the integers (6) and

$$H^*, K^*, L^* \qquad (11)$$

fulfil (7) as well as

$$\begin{vmatrix} H & K & L \\ H' & K' & L' \\ H^* & K^* & L^* \end{vmatrix}^2 = 1\,, \qquad (12)$$

$$0 \le 2W \le V \le V' \qquad (13)$$

(such integers (6), (11) do exist). Then (1) [or (2)] are standard p.m.d. of the planes $(h\,k\,l)$ with respect to fundamental cells [or with respect to meshes].

Algorithm

1. We find integers (6) in any way such that (7) and (8) hold. This may be done, *e.g*, as follows. If $h=0$, then

$$H=0,\ K=l,\ L=-k,\ H'=-1,\ K'=0,\ L'=0\,.$$

If $h \ne 0$, we put

$$L=\mathrm{HCF}(h,k),\ H'=k/L,\ K'=-h/L,\ L'=0 \quad (14)$$

and find the integer K so that

$$H=(l+KH')/K' \qquad (15)$$

is also an integer. For this purpose it is sufficient to test the values

$$0,\ l,\ 2l,\ \ldots,\ (|K'|-1)l$$

as K. Having found integers (6) we determine V.

0 Now V' and W are calculated. If $V > V'$, the numbers H, K, L, V are relabelled H', K', L', V', respectively, and *vice versa*. **1** If

$$2|W| \le V \qquad (16)$$

is not true, we put $m=[W/V+\frac{1}{2}]$, **2** relabel the values $H'-mH$, $K'-mK$, $L'-mL$ by H', K', L' respectively, and **3** return to the place **0**.

If (16) is correct, (10) is valid for the fundamental cells of N and Table 2 determines the shape and size of the meshes of N.

2. If interested in the parameters of the mutual displacement, we proceed as follows. If $W<0$, the numbers

$$H, K, L, W \qquad (17)$$

must be relabelled

$$-H, -K, -L, -W, \qquad (18)$$

respectively. We find in any way integers (11) fulfilling (12). This may be done for example as follows. Let

$$h^*=KL'-LK',\ k^*=LH'-HL',\ l^*=HK'-KH'\,.$$

If $h^*=k^*=0$, put $H^*=0$, $K^*=0$, $L^*=1$. If $h^*=0$, $k^* \ne 0$, put $H^*=0$ and find an integer L^* such that $K^*=-(1+l^*L^*)/k^*$ is also an integer; it is enough to test the values $0, 1, \ldots, |k^*|-1$ as L^*. If $h^* \ne 0$, integers K^*, L^* are to be found in such a way that $H^*=-(1+k^*K^*+l^*L^*)/h^*$ is again an integer. Here it is sufficient to examine independently the values

$$0, 1, \ldots, |h^*|/\mathrm{HCF}(h^*, k^*)-1$$

and

$$0, 1, \ldots, |h^*|/\mathrm{HCF}(h^*, l^*)-1$$

as K^* and L^*, respectively. Having found integers (11) we calculate U, U', Y, T_1, T_2 and (1) [or (2)] the latest triplet (1) [or (2)] being the standard p.m.d. of the planes $(h\,k\,l)$ with respect to fundamental cells [or with respect to meshes].

Remark

Equation

$$\begin{aligned} p^2q^2\sin^2\psi &= x^2y^2\sin^2\varphi \\ &= h^2b^2c^2\sin^2\alpha+k^2a^2c^2\sin^2\beta+l^2a^2b^2\sin^2\gamma \\ &\quad +2hkabc^2(\cos\alpha\cos\beta-\cos\gamma) \\ &\quad +2hlab^2c(\cos\alpha\cos\gamma-\cos\beta) \\ &\quad +2kla^2bc(\cos\beta\cos\gamma-\cos\alpha) \end{aligned}$$

may be used for checking the calculations.

4. Examples

Here (3) have the same meaning as in § 2, § 3. The numbers (1) and (2) designate the standard p.m.d. of the planes $(h\,k\,l)$ with respect to fundamental cells and meshes, respectively. Remember that – unlike (3) – they are not uniquely determined. In particular, if τ_1, τ_2, τ_3 are positive standard p.m.d., then $1-\tau_1, 1-\tau_2, \tau_3$ are also standard p.m.d. The calculations are left to the reader.

1. *Plane* (157) *in a primitive cubic lattice*. Fundamental cell: shape **P**, $p=\sqrt{6}$, $q=\sqrt{14}$, $\cos\psi=\sqrt{21}/14$, $t_1=$

19/75, $t_2=12/75$, $t_3=\sqrt{3}/15$. Mesh: shape **D**, $x=y=\sqrt{14}$, $\cos\varphi=11/14$, $t'_1=56/75$, $t'_2=31/75$, $t'_3=\sqrt{3}/15$.

2. *Plane* (421) *in a face-centred cubic lattice*. The conventional unit cell being not primitive we choose a primitive one, *e.g.* that with $a'=b'=c'=a\sqrt{2}/2$, $\cos\alpha'=\cos\beta'=\cos\gamma'=1/2$. Then the Miller indices transform as follows: $h'=(k+l)/d$, $k'=(h+l)/d$, $l'=(h+k)/d$ where $d=$ HCF $(k+l,h+l,h+k)$. Thus $h'=3$, $k'=5, l'=6$. The fundamental cell as well as the mesh are shaped **R** with $p=x=(\sqrt{6}/2)a$, $q=(\sqrt{14}/2)a$, $t_1=t'_1=1/6$, $t_2=t'_2=5/14$, $t_3=t'_3=(\sqrt{21}/42)a$.

3. *Plane* (012) *in a rhombohedral lattice* ($a=b=c$, $\cos\alpha=\cos\beta=\cos\gamma$). The shape depends on the parameter $\xi=\cos\alpha$ satisfying $-\frac{1}{2}<\xi<1$. A detailed discussion of the meshes based on inequalities (9) yields the following results:

(*a*) $\xi=0$ (this is actually the case of a primitive cubic lattice): **R**, $x^2=a^2$, $y^2=5a^2$, $t'_1=0$, $t'_2=\frac{2}{5}$.

(*b*) $0<|\xi|<\frac{1}{2}$: **P**, $x^2=a^2$, $y^2=(5-4\xi)\,a^2$, $\cos^2\varphi=\xi^2/(5-4\xi)$, $t'_1=3|\xi|/(\xi+5)$, $t'_2=(\xi+2)/(\xi+5)$.

(*c*) $\xi=\frac{1}{2}$: **D**, $x^2=y^2=3a^2$, $\cos^2\varphi=(\frac{5}{6})^2$, $t'_1=t'_2=\frac{8}{11}$.

(*d*) $\frac{1}{2}<\xi<\frac{5}{6}$: **P**, $x^2=a^2$, $y^2=6(1-\xi)a^2$, $\cos^2\varphi=(1-\xi)/6$, $t'_1=3(1-\xi)/(\xi+5)$, $t'_2=(\xi+2)/(\xi+5)$.

(*e*) $\xi=\frac{5}{6}$: **D**, $x^2=y^2=a^2$, $\cos^2\varphi=(\frac{1}{6})^2$, $t'_1=\frac{3}{35}$, $t'_2=\frac{17}{35}$.

(*f*) $\frac{5}{6}<\xi<1$: **P**, $x^2=6(1-\xi)a^2$, $y^2=a^2$, $\cos^2\varphi=(1-\xi)/6$, $t'_1=3/(\xi+5)$, $t'_2=2(2\xi+1)/(\xi+5)$.

In all cases $t_3'^2=((-2\xi^2+\xi+1)/(\xi+5))a^2$.

4. *Plane* (123) *in a primitive orthorhombic lattice* ($\cos\alpha=\cos\beta=\cos\gamma=0$). The shape depends on two parameters $u=a^2/b^2$, $v=c^2/b^2$. The results (without p.m.d.) were presented in the introduction.

5. Proofs

Let the assumptions of § 3 except the notation (5) be satisfied. Then vectors $\mathbf{a},\mathbf{b},\mathbf{c}$ may be found that $U\in[\mathbf{a},\mathbf{b},\mathbf{c}]_M$, $|\mathbf{a}|=a, \mathbf{a}\,.\,\mathbf{b}=ab\cos\gamma, \ldots.$

Lemma 1.

If $2|\mathbf{v}\,.\,\mathbf{v}'|\le\mathbf{v}^2\le\mathbf{v}'^2$ holds and $[\mathbf{v},\mathbf{v}']_N$ are primitive, then they are also fundamental.

Lemma 2

Let $|\mathbf{v}|\le|\mathbf{v}'|$, $2|\mathbf{v}\,.\,\mathbf{v}'|>\mathbf{v}^2$. Then, denoting $m=[\mathbf{v}\,.\,\mathbf{v}'/\mathbf{v}^2+\frac{1}{2}]$, inequalities

$$|\mathbf{v}'-m\mathbf{v}|<|\mathbf{v}'|\,,\quad |\mathbf{v}'-m\mathbf{v}|\le|\mathbf{v}'-n\mathbf{v}|$$

hold for every integer n.

The proofs of these two lemmas are left to the reader.

Proof of theorem 1

Suppose the integers (6) fulfil (7), (8), (9). Then integers H'',K'',L'' may be found so that

$$\begin{vmatrix} H & K & L \\ H' & K' & L' \\ H'' & K'' & L'' \end{vmatrix} = 1\,. \tag{19}$$

(Here the following theorem well known from algebra, the use of which will be made in this paragraph several times, has been applied: *if HCF* $(a_1,\ldots,a_n)=1$, *then integers* $x_1,\ldots,x_n$ *exist in such a way that* $a_1x_1+\ldots+a_nx_n=1$.) Let

$$\mathbf{v}\ =H\mathbf{a}+K\mathbf{b}+L\mathbf{c} \tag{20a}$$
$$\mathbf{v}'\ =H'\mathbf{a}+K'\mathbf{b}+L'\mathbf{c} \tag{20b}$$
$$\mathbf{v}''=H''\mathbf{a}+K''\mathbf{b}+L''\mathbf{c} \tag{20c}$$

so that

$$\mathbf{v}^2=V\,,\quad \mathbf{v}'^2=V'\,,\quad \mathbf{v}\,.\,\mathbf{v}'=W\,. \tag{21}$$

Any lattice vector $\mathbf{w}$ of M can be written

$$\mathbf{w}=r\mathbf{a}+s\mathbf{b}+t\mathbf{c}\quad (r,s,t \text{ integers}) \tag{22}$$

since the cell U is primitive. It may also be written

$$\mathbf{w}=q\mathbf{v}+q'\mathbf{v}'+q''\mathbf{v}''\quad (q,q',q'' \text{ integers})$$

where

$$q''=\begin{vmatrix} H & K & L \\ H' & K' & L' \\ r & s & t \end{vmatrix} \tag{23}$$

because of (20) and (19). If, in particular, $\mathbf{w}$ is a lattice vector of N, then

$$hr+ks+lt=0\,; \tag{24}$$

(7), (24) and (23) imply $q''=0$ since h,k,l are not all equal to zero. Thus any lattice vector $\mathbf{w}$ of N may be written $\mathbf{w}=q\mathbf{v}+q'\mathbf{v}'$ (q,q' integers), which means that $[\mathbf{v},\mathbf{v}']_N$ are primitive unit cells of N. According to (21), (9) and lemma 1 they are fundamental, too. Thus (10) is clear and Table 2 is an immediate consequence of Table 1. Theorem 1 has been proved with the exception of the note that integers (6) exist.

Proof of theorem 2

Suppose the integers (6), (11) fulfil (7), (12), (13). Let (20*a*, *b*) and $\mathbf{v}^*=H^*\mathbf{a}+K^*\mathbf{b}+L^*\mathbf{c}$ hold so that (21) and

$$\mathbf{v}\,.\,\mathbf{v}^*=U\,,\quad \mathbf{v}'\,.\,\mathbf{v}^*=U' \tag{25}$$

are true. The assumptions of theorem 1 being fulfilled, $[\mathbf{v},\mathbf{v}']_N$ are fundamental cells of N. According to (13), $|\mathbf{v}|\le|\mathbf{v}'|$, $\mathbf{v}\,.\,\mathbf{v}'\ge0$ so that $|\mathbf{v}|=p$, $|\mathbf{v}'|=q$, $\mathbf{v}\,.\,\mathbf{v}'=pq\cos\psi$ and consequently

$$\mathbf{v}^2\mathbf{v}'^2-(\mathbf{v}\,.\,\mathbf{v}')^2=p^2q^2\sin^2\psi\ne0\,. \tag{26}$$

Any lattice vector (22) of M can be also written

$$\mathbf{w}=q\mathbf{v}+q'\mathbf{v}'+q^*\mathbf{v}^*\quad (q,q',q^* \text{ integers})$$

because of (12); this means that the unit cells $[\mathbf{v},\mathbf{v}',\mathbf{v}^*]_M$ are primitive. Thus choosing a point $O\in N$ the point $O+\mathbf{v}^*$ lies in the neighbouring plane $(h\ k\ l)$. Let us introduce the vector $\mathbf{k}$ for which

$$|\mathbf{k}|=1\,,\quad \mathbf{v}\,.\,\mathbf{k}=\mathbf{v}'\,.\,\mathbf{k}=0 \tag{27}$$

is valid. Then real numbers T_1, T_2, T_3 fulfilling

$$\mathbf{v}^* = T_1\mathbf{v} + T_2\mathbf{v}' + T_3\mathbf{k} \tag{28}$$

are clearly p.m.d. of the planes $(h\ k\ l)$ with respect to fundamental cells; (27) and (28) imply

$$\begin{aligned} \mathbf{v} \ . \ \mathbf{v}^* &= T_1\mathbf{v}^2 + T_2\mathbf{v} \ . \ \mathbf{v}' \\ \mathbf{v}' \ . \ \mathbf{v}^* &= T_1\mathbf{v} \ . \ \mathbf{v}' + T_2\mathbf{v}'^2 \end{aligned}$$

from which (5) follows [see (26), (21), (25)]. The volume of any primitive cell of M is clearly $|T_3|\ pq \sin \psi = |T_3|\sqrt{Y}$ [see (26), (21), (4)] as well as $abc\sqrt{X}$, this expression being well known from elementary crystallography; thus $|T_3| = abc\sqrt{X/Y}$. Now it is evident that (1) are standard p.m.d. of the planes $(h\ k\ l)$ with respect to fundamental cells. If $2W = V < V'$ is fulfilled, then $[\mathbf{v}'-\mathbf{v},\ \mathbf{v}']_N$ are meshes of N and $|\mathbf{v}'-\mathbf{v}| = |\mathbf{v}'|$, $(\mathbf{v}'-\mathbf{v}) \ . \ \mathbf{v}' > 0$ is true; this can be easily verified. Accordingly in this case $-t_1, t_1+t_2, t_3$ are p.m.d. and consequently (2) are the standard p.m.d. of the planes $(h\ k\ l)$ with respect to meshes. The other cases are trivial. Thus the proof of the theorem 2 is completed, but the existence of the integers (6), (11) is not yet guaranteed.

Proof of the algorithm

1. First we are seeking integers (6) fulfilling (7), (8). The case $h=0$ is trivial. If $h \neq 0$ and (14) holds, H', K' $(K' \neq 0)$ are without common factor and according to the above algebraic theorem integers $\bar{H}$, $\bar{K}$ exist such that $\bar{H}K' - \bar{K}H' = 1$. In other words an integer $\bar{K}$ exists such that $(1+\bar{K}H')/K'$ is an integer, too. Since in this case $(1+(\bar{K}+iK')H')/K'$ (i integer) are integers as well, it is possible to find $\bar{K}$ with the required property among $|K'|$ subsequent integers, *e.g.* $0, 1, \ldots, |K'|-1$. Putting $H = l\bar{H}$, $K = l\bar{K}$, (15) is true. Then it is easy to verify that integers (6) found in this way fulfil (7), (8).

Now we have come in the algorithm to the cycle which may be repeated several times. If the values (6) satisfy conditions (7), (8) at the point **0**, then they do so also at the point **1**. If the values (6) satisfy conditions (7), (8) when entering the cycle for the ith $(i \geq 1)$ time, they satisfy them also when entering it for the $(i+1)$th time – if doing that at all. Thus conditions (7), (8) are always fulfilled since they are on the first time. Accordingly as soon as inequality (16) is found to be correct, we interrupt the cycle and apply theorem 1 following the directions of the algorithm. We have only to show that this situation actually occurs at some time (*i.e.* after a finite number of these cycles).

Let us use notation (20*a*, *b*). Assuming that during the ith cycle inequality (16) is not satisfied, we get

$$|\mathbf{v}| \leq |\mathbf{v}'|\ , \quad 2|\mathbf{v} \ . \ \mathbf{v}'| > \mathbf{v}^2\ , \quad m = [\mathbf{v} \ . \ \mathbf{v}'/\mathbf{v}^2 + \tfrac{1}{2}]$$

taking the instantaneous values at **2**. According to lemma 2 $|\mathbf{v}' - m\mathbf{v}| < |\mathbf{v}'|$. But the vector $\mathbf{v}' - m\mathbf{v}$ subsequently changes its notation to $\mathbf{v}'$ at **3**. That means that the value of the sum $|\mathbf{v}| + |\mathbf{v}'|$ when entering the cycle for the $(i+1)$th time is smaller than it was when entering it for the ith time. But $\mathbf{v}$, $\mathbf{v}'$ are *lattice* vectors of M. Thus the first part of the algorithm and the existence of the integers (6) from theorem 1 is proved. Notice that the choice of the number m was the best in the sense that choosing it in another way we could never get a shorter vector $\mathbf{v}' - m\mathbf{v}$ (see the second inequality in lemma 2).

2. Relabelling, if $W < 0$, the numbers (17) by (18) conditions (7), (8), (13) are satisfied. Integers (11) fulfilling (12) exist according to the quoted algebraic theorem. It is not difficult to show that they may be found in the way given in the algorithm.

Proof of the remark follows immediately from the well known relations of elementary crystallography.

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