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The Geometry of Lattice Planes

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A simple method is outlined for finding the arrangement of lattice points in a lattice plane of given Miller indices, and for determining the stacking properties of such planes.

Introduction

In a recent paper Neustadt, Cagle & Waser (1968) indicated the usefulness of the reciprocal lattice as an aid to the solution of problems in lattice geometry. No reference was made however to recent papers describing elegant and general solutions to problems in lattice geometry which result when the concept of the reciprocal lattice is used in conjunction with a tensor notation. General descriptions of the type of problem which may be solved in this way are given by Patterson (1959) and Rautala, Guy & Smith (1964), and examples of more detailed analyses are given in recent papers on the crystallography of deformation twinning by Bilby & Crocker (1965), Saxl (1967) and Bevis & Crocker (1968). Further examples are given below in the form of alternative solutions to those given by Jaswon & Dove (1955) and Jaswon (1965) to problems on the geometry of lattice planes. These problems are relevant to the recent interest in the interpretation of electron diffraction patterns from twinned crystalline foils (Bullough & Wayman, 1966; Calbick & Marcus, 1967).

In this analysis, lattice vectors and reciprocal-lattice vectors representing lattice-plane normals will be referred to the direct lattice basis $\mathbf{c}_i$ ($i=1,2,3$) and the reciprocal lattice basis $\mathbf{c}^i$ respectively. The direct and reciprocal lattice bases are related by the equations $\mathbf{c}^i.\mathbf{c}_j = \delta^i_j$, $\mathbf{c}^i = c^{ij}\mathbf{c}_j$ or $\mathbf{c}_i = c_{ij}\mathbf{c}^j$ where δ^i_j is the Kronecker delta, $c_{ij} = \mathbf{c}_i \,.\, \mathbf{c}_j$ and $c^{ij} = \mathbf{c}^i \,.\, \mathbf{c}^j$ are the metric tensors of the direct and reciprocal lattice bases respectively, and the summation convention of the tensor calculus applies. The lattice vector $\mathbf{v}$ parallel to the direction with indices $[v^i]$ and the vector $\mathbf{h}$ normal to the plane with Miller indices (h_i) will be represented by vectors $\mathbf{v}=v^i\mathbf{c}_i$ and $\mathbf{h}=h_i\mathbf{c}^i$ respectively. The indices $[v^i]$ are the contravariant components v^i of the vector $\mathbf{v}$ and the Miller indices (h_i) are the covariant components h_i of the vector $\mathbf{h}$.

Arrangement of lattice points in a lattice plane

The problem of mapping a lattice plane with Miller indices (h_i) is considered first. Let the vectors $\mathbf{u}=u^i\mathbf{c}_i$ and $\mathbf{v}=v^i\mathbf{c}_i$ (Fig. 1) be primitive lattice vectors which define a cell in the lattice plane (h_i), so that $h_iu^i=h_iv^i=0$, and let the vector $\mathbf{w}=w^i\mathbf{c}_i$ be a primitive lattice vector joining a lattice point in the plane (h_i) containing the origin (plane 0) to a lattice point in the next parallel plane (plane 1), so that $h_iw^i=1$. If the lattice parameters as described by $\mathbf{c}_i$ are known, then c_{ij} and c^{ij} can be calculated. The cell defined by $\mathbf{u}$ and $\mathbf{v}$ may then be constructed, since u and v, the magnitudes of $\mathbf{u}$ and $\mathbf{v}$ respectively, are given by the equations:

$$u^2=c_{ij}u^iu^j\,;\quad v^2=c_{ij}v^iv^j\,, \tag{1}$$

and the angle φ between $\mathbf{u}$ and $\mathbf{v}$ is given by

$$\cos\varphi=(c_{ij}u^iv^j)u^{-1}v^{-1}\,. \tag{2}$$

If a plane is to be mapped correctly, then it is essential that $\mathbf{u}$ and $\mathbf{v}$ define a primitive cell in that plane. A simple rule which ensures that the components u^i and v^i are the components of vectors defining a primtive cell in a lattice plane may be derived as follows.

The case where $\mathbf{c}_i$ defines a primitive cell is considered first. The volume V' of the cell defined by $\mathbf{u}$, $\mathbf{v}$ and $\mathbf{w}$ is equal to

$$V'=\mathbf{h}\,.\,\mathbf{u}\times\mathbf{v}\,, \tag{3}$$

where $\mathbf{h}$ is the vector normal to $\mathbf{u}$ and $\mathbf{v}$, with magnitude

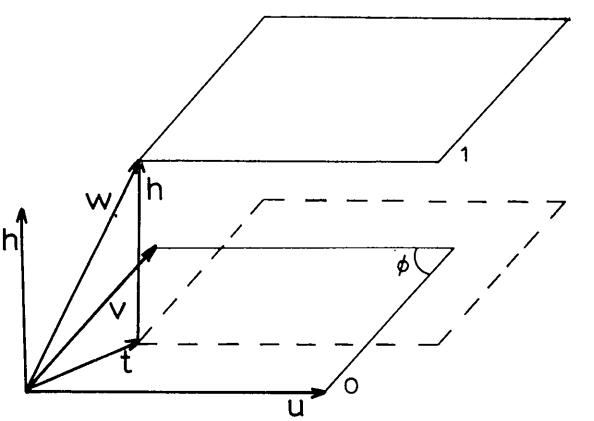

Fig. 1. Illustration of vectors $\mathbf{u}$, $\mathbf{v}$, $\mathbf{w}$, $\mathbf{h}$ and $\mathbf{t}$. The vectors $\mathbf{u}$ and $\mathbf{v}$ define a plane with Miller indices (h_i). The plane (0) contains the origin and plane (1) is the next parallel plane.

$(c^{ij}h_ih_j)^{-\frac{1}{2}}$ equal to the interplanar spacing of planes (h_i),

$$\mathbf{h}=h_i\mathbf{c}^i(c^{ij}h_ih_j)^{-1}\,. \tag{4}$$

The vector product of $\mathbf{u}$ and $\mathbf{v}$ is equal to

$$\mathbf{u}\times\mathbf{v}=Vk_i\mathbf{c}^i\,, \tag{5}$$

where V is the volume of the cell defined by the basis $\mathbf{c}_i$ and

$$k_i=\varepsilon_{jki}u^jv^k\,. \tag{6}$$

ε_{jki} $(i,j,k=1,2,3)$ are the components of the alternating tensor. Substituting equations (4) and (5) in equation (3) we obtain

$$V'=Vc^{ij}k_ih_j(c^{ij}h_ih_j)^{-1}\,. \tag{7}$$

If the cell defined by $\mathbf{c}_i$ is a primitive cell then the cell defined by $\mathbf{u}$, $\mathbf{v}$ and $\mathbf{w}$ is also primitive when $V=V'$, and in this case equation (7) reduces to

$$c^{ij}h_ih_j=c^{ij}k_ih_j\,. \tag{8}$$

The general solution to equation (8) is $k_i=h_i$, so that the restriction on u^i and v^i which ensures that $\mathbf{u}$ and $\mathbf{v}$ define a primitive cell in the lattice plane (h_i) is given by

$$h_i=\varepsilon_{jki}u^jv^k\,. \tag{9}$$

The components v^i of lattice vectors contained in the plane (h_i) may be generated from the components of any primitive lattice vector $u^i\mathbf{c}_i$ contained in this plane using the relation

$$[v^i]=[u^1-h_3m_2+h_2m_3\,,\ u^2+h_3m_1-h_1m_3\,,\ u^3-h_2m_1+h_1m_2]\,, \tag{10}$$

where m_1, m_2 and m_3 are arbitrary integers. Equations (9) and (10) give the following restriction on the integers m_1, m_2 and m_3.

$$m_1u^1+m_2u^2+m_3u^3=1\,, \tag{11}$$

which ensures that $u^i\mathbf{c}_i$ and $v^i\mathbf{c}_i$ define a primitive cell in the plane (h_i). The procedure for determining integral solutions (m_1,m_2,m_3) of this linear diophantine equation is straightforward; see for example Hunter (1964). Substitution in equation (10) of a solution (m_i') of equation (11) or any solution obtained from the general solution of equation (11) in the form

$$m_i=m_i'-\varepsilon_{jki}u^jn_k\,,$$

$(n_1,n_2,n_3$ arbitrary integers) will give the components v^i of a vector $\mathbf{v}$.

The most direct method of mapping a lattice plane with Miller indices (h_1,h_2,h_3) is to take $u^i\mathbf{c}_i$ to be one of the lattice vectors with components $d^{-1}[0h_3\bar{h}_2]$, $d^{-1}[h_30\bar{h}_1]$ or $d^{-1}[h_2\bar{h}_10]$, where d is the highest common factor of the two non-zero components $[u^i]$. For example, for $(h_i)=(433)$ these three lattice vectors are $[01\bar{1}]$, $d=3$; $[30\bar{4}]$, $d=1$; $[3\bar{4}0]$, $d=1$. For the case $[u^i]=[h_2\bar{h}_10]$ equation (11) becomes

$$m_1h_2-m_2h_1=1\,, \tag{12}$$

and by equation (10) the solution (m_1,m_2) of equation (13) results in the following components for the vector $\mathbf{v}$

$$[v^i]=[h_2(1+m_3)-h_3m_2\,,\ -h_1(1+m_3)+h_3m_1\,,\ -1]\,, \tag{13}$$

where m_3 is an arbitrary integer. Further vectors $\mathbf{v}$ may be generated by using the general solution for equation (12). A solution (m_1,m_2) of equation (12) may be determined rapidly by inspection. For example, if the greater of $|h_1|$ and $|h_2|$ is equal to T, then for $2\leq T\leq 20$, values of $|m_1|$ and $|m_2|$ can always be less than or equal to $\left(\frac{T+1}{2}-1\right)$ or $\left(\frac{T}{2}-1\right)$, for T odd or even respectively. The exception is for the case when one of $|h_1|$ or $|h_2|$ is unity, where in any case the solution of equation (12) is trivial. Analogous procedures apply when the components of the vector $\mathbf{u}$ are taken to be $[0h_3\bar{h}_2]$ or $[h_30\bar{h}_1]$.

The extension of the analysis given above to cases where the basis $\mathbf{c}_i$ defines a centred cell is trivial. For lattice planes with Miller indices satisfying the conditions given in Table 1 the number p is the number of the vectors $\mathbf{u}$, $\mathbf{v}$ and $\mathbf{u}+\mathbf{v}$ which must be doubly primitive centred lattice vectors. The correct mapping is obtained by reducing the magnitudes of the relevant vectors by one half.

Table 1. *Details of the way cell centring changes the arrangement of lattice points in a lattice plane and the stacking properties of such planes*

Cell	Type of plane	p	q
Primitive	$h_1h_2h_3$	0	0
Body-centred	$h_1+h_2+h_3$ even	1	0
	$h_1+h_2+h_3$ odd	0	1
Face-centred	h_1, h_2, h_3 all odd	2 (3)	0
	h_1, h_2, h_3 mixed	1	1
Base centred	h_1+h_2 even	1	0
($\mathbf{c}_3$)	h_1+h_2 odd	0	1

Stacking properties of lattice planes

The determination of the stacking properties of lattice planes with Miller indices (h_i) is considered next, and is restricted at first to cases where $\mathbf{c}_i$ defines a primitive cell. The projection of plane 1 onto plane 0 is indicated by broken lines in Fig. 1. The shift vector $\mathbf{t}$ (Jaswon & Dove, 1955) which enables the stacking properties of

the planes (h_i) to be determined is equal to $\mathbf{t}=\mathbf{w}-\mathbf{h}$. On noting that

$$\mathbf{h}=h^i\mathbf{c}_i=h_i\mathbf{c}^i \text{ where } h^i=c^{ij}h_j\,,$$

then

$$\mathbf{t}=[w^i-h^i(h^kh_k)^{-1}]\mathbf{c}_i=t^i\mathbf{c}_i\,. \qquad (14)$$

The magnitude of $\mathbf{t}$ and the angle between $\mathbf{t}$ and $\mathbf{u}$ or $\mathbf{v}$ may be determined from equations analogous to equations (1) and (2) and hence the stacking properties of the (h_i) planes determined. When $\mathbf{c}_i$ defines a centred cell the magnitude of $\mathbf{t}$ must be reduced by one half when q of Table 1 is equal to 1, and remains as for the primitive case when $q=0$.

The analysis presented above may be used for studying the geometry of lattice planes in any lattice provided that the lattice parameters of the basis $\mathbf{c}_i$ are known, and that the basis $\mathbf{c}_i$ defines one of the centred cells indicated in Table 1. The analysis is clearly applicable to the study of reciprocal lattice planes and may also be extended without difficulty to include the mapping of motif units.

Application

In this section the analyses presented above are used to map and determine the stacking properties of the (5,8,11) body-centred cubic lattice planes which have been predicted as likely deformation twin habit planes in b.c.c. crystals (Bevis, Rowlands & Acton, 1968). In the mapping of the (5,8,11) plane the components of the vector $u^i\mathbf{c}_i$ are taken to be $[8\bar{5}0]$. For this case equation (13) is equal to

$$8m_1-5m_2=1\,.$$

An integral solution (m_1,m_2) of this equation is (2,3) and a selection of vectors $\mathbf{v}$ which, together with $[u^i]=[8\bar{5}0]$ define a primitive cell in the (5,8,11) lattice plane, are given by equation (13) as:

$$[v^i]=[8(1+m_3)-33\,,\ -5(1+m_3)+22\,,\ -1]$$

where m_3 is an arbitrary integer. For example, for $m_3=0$, 1, 2 and 3 the components $[v^i]$ are $[\bar{2}5,17,\bar{1}]$, $[\bar{1}7,12,\bar{1}]$, $[\bar{9},7,\bar{1}]$ and $[\bar{1}2\bar{1}]$ respectively. Equations (1) and (2) have been used to determine the dimensions of the cell defined by $[8\bar{5}0]$ and $[\bar{1}2\bar{1}]$ and the resultant cell is shown in bold lines in Fig. 2. Reference to Table 1 for the (5,8,11) plane gives $p=1$ so that one of the vectors $\mathbf{u}$, $\mathbf{v}$ or $\mathbf{u}+\mathbf{v}$ must be a doubly primitive b.c.c. lattice vector. In this case $\mathbf{u}+\mathbf{v}$ is doubly primitive so that the cell in Fig. 2 is centred.

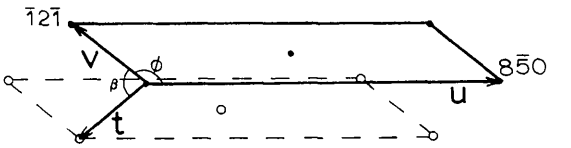

Fig. 2. The body-centred cubic (5, 8, 11) lattice plane. $u=(89)^{1/2}a$, $v=(6)^{1/2}a$ and $\cos\varphi=-18/(6\times89)^{1/2}$ where a is the lattice parameter of the body-centred cubic cell. $t=(22\ 02\ 90)^{1/2}\,.\,a/210$, $\cos\beta=210/(22\ 02\ 90\times6)^{1/2}$ and the open circles represent the projection of lattice points in plane (1) onto plane (0).

In determining the stacking properties of lattice planes (h_i) it is necessary to choose a lattice vector $\mathbf{w}=w^i\mathbf{c}_i$ which joins the origin (plane 0) to a lattice point in the next parallel plane (plane 1). The restriction on the components w^i is $h_iw^i=1$. For the (5,8,11) planes the components $[w^i]$ have been taken to be $[\bar{2}01]$. The quantities $[h^i(h^kh_k)^{-1}]$ in equation (14) are equal to $(210)^{-1}$ [5,8,11], so that the shift vector $\mathbf{t}$, by equation (14), has components $[t^i]=(210)^{-1}[-425,-8,199]$. From Table 1, $q=0$ for the (5,8,11) b.c.c. lattice plane so that this is a shift vector of the correct magnitude and is indicated in Fig. 2.

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