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The Geometry of Lattice Planes. I

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A simple but powerful 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. The theory is extended to cover the case of motif points within the primitive unit cell.

Introduction

In this paper we take up the formal mathematical problem of finding the arrangement of lattice points in a lattice plane of given Miller indices (*hkl*). The problem does not admit of a general algebraic solution in terms of h, k and l, but it is possible to lay down a simple procedure for determining a pair of primitive translation vectors for the plane in any given case. When one of the indices is unity, e.g. (*hk*1), a solution may be found in terms of the other two (here h and k). The arrangement of lattice points is the same for all lattice planes of given (*hkl*), but the vector joining any lattice point to the nearest lattice point in the next plane of the series has in general a component parallel to the plane. This component, referred to hereafter as the shift vector, determines all the stacking properties of the series. The problem of determining the shift vector admits of a solution subject to the same limitations as that of the preceding problem. The analysis is readily extended to cover the case of motif points within the unit cell. A search through the crystallographic literature has failed to reveal any previous general attack on these problems, though a number of particular cases have been treated by intuitive methods not requiring formal algebraic procedures. We hope that our techniques will prove of use to a fairly wide class of reader and therefore, in the interests of generality and conciseness, we omit all consideration of possible applications. These include the analysis of habit planes occurring in martensite transformations, a novel crystallographic treatment of atomic movements in deformation twinning and the determination of the structure of edge dislocations in crystals, and will be taken up in two papers forthcoming.

Arrangement of lattice points in a lattice plane

Let three vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$, of lengths a, b, c respectively, constitute a set of primitive translation vectors for a lattice. Any triplet of integers u, v, w then defines a lattice point, or vector $u\mathbf{a}+v\mathbf{b}+w\mathbf{c}$, the triplet u, v, w being referred to as the co-ordinates of the point. The plane of Miller indices (*hkl*) passing through the origin has the equation

$$hu+kv+lw = 0\,,$$

so that it certainly passes through the lattice points

$$0, 0, 0;\ l, 0, \bar{h};\ 0, l, \bar{k};\ \text{and}\ k, \bar{h}, 0\,.$$

In the present discussion it is assumed that h, k, l are all relatively prime, the more general case introducing only minor complications which can be treated by an extension of the present methods. It will be appreciated that the vectors

$$\mathbf{a}' = l\mathbf{a}-h\mathbf{c},\ \mathbf{b}' = l\mathbf{b}-k\mathbf{c}$$

illustrated in Fig. 1 do not necessarily constitute a pair of primitive translation vectors for the plane

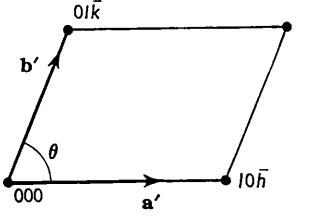

Fig. 1. Illustration of vectors $\mathbf{a}' = l\mathbf{a}-h\mathbf{c}$, $\mathbf{b}' = l\mathbf{b}-k\mathbf{c}$ lying in the plane of indices (*hkl*).

$$a' = |l\mathbf{a}-h\mathbf{c}|,\ b' = |l\mathbf{b}-k\mathbf{c}|,\ \cos\theta = \mathbf{a}'\cdot\mathbf{b}'/a'b'.$$

$hu+kv+lw = 0$, and that, indeed, the question of their status constitutes the kernel of the problem. To investigate this point we set up a new system of axes defined by $\mathbf{a}'$, $\mathbf{b}'$, and a vector $\mathbf{c}'$ perpendicular to the plane and of arbitrary length, so that any vector $u\mathbf{a}+v\mathbf{b}+w\mathbf{c}$ is relabelled into the form $u'\mathbf{a}'+v'\mathbf{b}'+w'\mathbf{c}'$, where the new co-ordinates u', v', w' are not necessarily integers. It is convenient to write

$$\mathbf{c}' = p\mathbf{a}+q\mathbf{b}+r\mathbf{c}\,,$$

where p, q, r are sufficiently defined by

$$\mathbf{c}'\cdot\mathbf{a}' = \mathbf{c}'\cdot\mathbf{b}' = 0$$

(and are not necessarily integers). Now, substituting for $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ in the equation

$$u\mathbf{a}+v\mathbf{b}+w\mathbf{c} = u'\mathbf{a}'+v'\mathbf{b}'+w'\mathbf{c}'\,,$$

we obtain at once the co-ordinate transformation

$$\begin{Bmatrix} u \\ v \\ w \end{Bmatrix} = \begin{Bmatrix} l & 0 & p \\ 0 & l & q \\ \bar{h} & \bar{k} & r \end{Bmatrix} \begin{Bmatrix} u' \\ v' \\ w' \end{Bmatrix}. \qquad (1)$$

We are particularly interested in applying (1) to a lattice point u_0, v_0, w_0 in the plane

$$hu+kv+lw = 0$$

(i.e. a lattice point for which necessarily $w' = 0$), in which case

$$u_0 = lu'; \; v_0 = lv'; \; w_0 = \bar{h}u'+\bar{k}v' ,$$

i.e.

$$u' = (1/l)u_0; \; v' = (1/l)v_0; \; w' = 0; \; l \neq 0 . \qquad (2)$$

If $u_0 = N_1 l$, $v_0 = N_2 l$, where N_1, N_2 are integers, then u', v' are integers defining lattice points at the corners of parallelograms, each of side $\mathbf{a}'$, $\mathbf{b}'$, as illustrated in Fig. 1.

Interior points are effectively defined by

$$1 \leqslant u_0 \leqslant l-1, \; 1 \leqslant v_0 \leqslant l-1 , \qquad (3)$$

there being $l-1$ such points in each parallelogram, as proved below and as illustrated in Fig. 2 for the plane

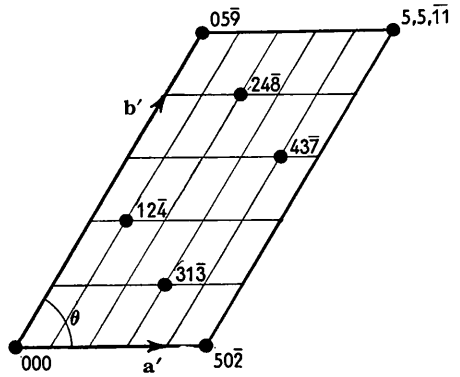

Fig. 2. Map of plane (295) in the primitive cubic lattice. $a' = \sqrt{29}$, $b' = \sqrt{106}$, $\cos\theta = 18/(\sqrt{29}\times 106)$.

(295) in the primitive cubic lattice; when $l = 1$ there are no interior points, thus proving that a', b' constitute a pair of primitive vectors for the plane $(hk1)$. Since h, k have the same status as l, it follows, by introducing $k, \bar{h}, 0$ in (1) in place of either $l, 0, \bar{h}$ or $0, l, \bar{k}$, that a pair of primitive vectors may also be obtained when $h = 1$, $k = 1$ respectively; either of these alternative transformations may be used if $l = 0$. The procedure for finding interior lattice points is in general as follows: set $u = 1$ and find a solution of $h+kv+lw = 0$ (this being always possible by virtue of Euclid's algorithm, bearing in mind that h, k, l are all relatively prime); if v, w is one such solution, then any other solution must necessarily have the form $v+nl$, $w-nk$, where n is any integer; by a suitable choice of n we may thus satisfy $1 \leqslant v_0 \leqslant l-1$, and hence (since $u = 1$ satisfies $1 \leq u_0 \leq l-1$) determine an interior point $1, v_0, w_0$ of the parallelogram. To prove that there are $l-1$ interior points, it suffices to remark that we can set $u = 2, 3, \ldots, l-1$ and repeat the procedure.

The shift vector

To investigate the shift vector, we note in the first place that all planes parallel to $hu+kv+lw = 0$ have the equation $hu+kv+lw = C$, where C is necessarily an integer. By assigning any integral value to w and noting that, by Euclid's algorithm, integers u and v may be found so that $hu+kv = 1-lw$, it follows that $C = 1$ is possible and that it defines the nearest parallel plane to the original plane (i.e. $C = 0$); similarly all other integral values are allowed for C. On working out the inverse of the transformation (1), applying it to the lattice point u_c, v_c, w_c in the plane $hu+kv+lw = C$, and collecting terms we obtain

$$u' = \frac{1}{l}\left(u_c - \frac{pC}{hp+kq+lr}\right), \quad v' = \frac{1}{l}\left(v_c - \frac{qC}{hp+kq+lr}\right),$$

$$w' = \frac{C}{hp+kq+lr}, \qquad (4)$$

where

$$\begin{pmatrix} p \\ q \\ r \end{pmatrix} = \begin{Bmatrix} (bc/a)(1-n_\alpha^2) & c(n_\alpha n_\beta - n_\gamma) & b(n_\gamma n_\alpha - n_\beta) \\ c(n_\alpha n_\beta - n_\gamma) & (ca/b)(1-n_\beta^2) & a(n_\beta n_\gamma - n_\alpha) \\ b(n_\gamma n_\alpha - n_\beta) & a(n_\beta n_\gamma - n_\alpha) & (ab/c)(1-n_\gamma^2) \end{Bmatrix} \begin{pmatrix} h \\ k \\ l \end{pmatrix}, \qquad (5)$$

on writing

$$n_\alpha = \frac{\mathbf{b}\cdot\mathbf{c}}{bc}, \quad n_\beta = \frac{\mathbf{c}\cdot\mathbf{a}}{ca}, \quad n_\gamma = \frac{\mathbf{a}\cdot\mathbf{b}}{ab}.$$

Setting $C = 0$ gives the relations (2) previously deduced directly.

It may be noted that u', v' in (4) depend only on the ratio $p:q:r$, in contrast to w'; distances along the z' direction are given by

$$w'c' = \frac{C}{hp+kq+lr} \cdot |p\mathbf{a}+q\mathbf{b}+r\mathbf{c}| , \qquad (6)$$

which again depends only on $p:q:r$. Setting $C = 1$ in (6) gives the interplanar spacing. Setting $C = 1$ in (4) gives the u', v', w' of a lattice point u_1, v_1, w_1 in the plane $hu+kv+lw = 1$, of which the projection on the plane $C = 0$ is $u', v', 0$; the join of u', v' to the most convenient neighbouring lattice point of $C = 0$ then defines the shift vector $\mathbf{t}$. In the general case it is necessary to obtain u_1, v_1, w_1 by inspection, but if $l = 1$ we see that an immediate solution is $u_1, v_1, w_1 = 0, 0, 1$ so that

$$u' = \frac{-p}{hp+kq+r}, \quad v' = \frac{-q}{hp+kq+r}; \qquad (7)$$

similar considerations apply if $h = 1$ or $k = 1$.

The symbol ○ in Fig. 3, of co-ordinates

$$\frac{108}{\bar{1}\bar{1}0}, \; \frac{101}{\bar{1}\bar{1}0}, \; \frac{\bar{2}\bar{2}\bar{5}}{\bar{1}\bar{1}0}$$

marks the projection of a lattice point in the (295) plane $C = 1$, i.e. the point $1, 1, \bar{2}$. If this projection

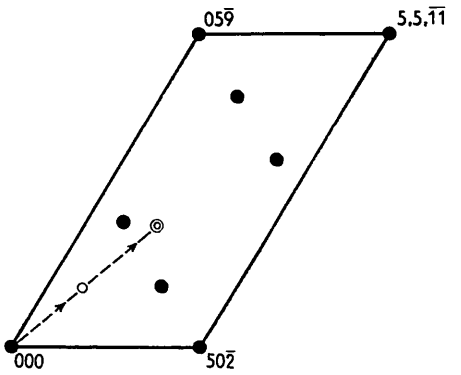

Fig. 3. Stacking of (295) planes in the primitive cubic lattice. The symbols ○, ◎ mark respectively the projection of lattice points lying in the two successive planes to the plane mapped, the heights of the points being d_{295}, $2d_{295}$ respectively.

is regarded as being obtained from the origin by a shift along the broken line, as indicated, then the shift vector is given by

$$\left[\frac{108}{110}, \frac{101}{110}, \frac{\overline{225}}{110}\right] - [0, 0, 0] = \left[\frac{108}{110}, \frac{101}{110}, \frac{\overline{225}}{110}\right].$$

A shift of double the amount leads to the point denoted by the symbol ◎, which marks the projection of a lattice point in $C = 2$; evidently the 110th projection obtained in this way will coincide with a lattice point of $C = 0$, thus showing that the stacking pattern of the primitive cubic (295) planes constitutes a congruence modulo 110. To prove that the stacking pattern of the primitive cubic (hkl) planes constitutes a congruence modulo $h^2+k^2+l^2$, we note:

(i) that the normal, through the origin, to the plane $hu+kv+lw = 0$, passes through h, k, l;

(ii) that there exist no lattice points between 0, 0, 0 and h, k, l along the direction of the normal;

(iii) that h, k, l lies on the plane $hu+kv+lw = h^2+k^2+l^2$;

(iv) and that there exists a series of equally spaced planes, defined by $C = 1, 2, \ldots$ between $C = 0$ and $C = h^2+k^2+l^2$.

Motif points

We now introduce a motif point B at a translation vector $x\mathbf{a}+y\mathbf{b}+z\mathbf{c}$ from each lattice point (referred to hereafter as an A-point), thus defining a second lattice (the B-lattice) interpenetrating the original (the A-lattice). This means that there exists a motif point B (B-point) within any primitive cell defined by A-points, and, in particular, at the position x, y, z within the cell defined by the primitive triplet $\mathbf{a}, \mathbf{b}, \mathbf{c}$. In relation to the series of parallel lattice planes $hu+kv+lw = C$ (the A-planes), there are two distinct possibilities for a B-point, namely:

(1) It lies on an A-plane, this being the case if $hx+ky+lz = C'$ is an integer; for if u, v, w are the co-ordinates of an A-point in the plane C, then $u+x$, $v+y$, $w+z$ are the co-ordinates of a B-point in the plane $C+C'$—which is an A-plane since $C+C'$ is an integer. The array of A- and B-points in the plane does not constitute a two-dimensional lattice, for there exists a motif point B within any primitive parallelogram defined by A-points. To find this two-dimensional motif, it suffices to determine the position of any B-point in the plane $C = 0$.

(2) It does not lie on an A-plane, this being the case if $hx+ky+lz = C'$ is not an integer. In this case it is convenient to write $C' = C+\delta$, where C is an integer and where $|\delta| < \frac{1}{2}$, and to associate the B-plane $C+\delta$ with the A-plane C, thus obtaining a series of parallel B-planes $\ldots\delta, 1+\delta, 2+\delta\ldots$ of indices (hkl), associated respectively with the A-planes $\ldots 0, 1, 2, \ldots$. It will be appreciated that we must now consider the shift vector $\mathbf{t}_{AB}$ relating C to $C+\delta$ in addition to the original shift vector $\mathbf{t}$ (now preferably re-written $\mathbf{t}_{AA}$, or, since the shift between successive B-planes is the same as between successive A-planes, $\mathbf{t}_{BB}$). The vector $\mathbf{t}_{AB}$ may be formally defined as the component, parallel to the plane (hkl), of the vector joining an A-point in the plane C to the nearest B-point in the plane $C+\delta$. This vector may be found as follows: the B-point x, y, z lies on the B-plane $C+\delta = hx+ky+lz$, so that its projection $x', y', 0$ on $C = 0$ is given by

$$x' = \frac{1}{l}\left\{x - \frac{p(hx+ky+lz)}{hp+kq+lr}\right\},$$

$$y' = \frac{1}{l}\left\{y - \frac{q(hx+ky+lz)}{hp+kq+lr}\right\};$$

since C, δ are known, we thus determine

$$x'\mathbf{a}'+y'\mathbf{b}'-C\mathbf{t}_{BB} \qquad (8)$$

as the projection on $C = 0$ of a B-point in the plane δ: the joint of this projection to the nearest A-point in $C = 0$ then defines $\mathbf{t}_{AB}$. When $\delta = 0$ the present case reduces to the preceding, and (8) gives the position of a B-point lying in $C = 0$.

If a lattice is described by a non-primitive unit cell (sometimes referred to as a structure cell), e.g. the b.c.c. lattice, it may be regarded as consisting of two interpenetrating lattices (i.e. an A-lattice and a B-lattice) for which the motif point B occupies a special position. As before there are two possibilities for a B-point, namely:

(1) It lies on an A-plane, in which case the array of A- and B-points in the plane constitutes a two-dimensional lattice.

(2) It does not lie on an A-plane, in which case necessarily

$\delta = \frac{1}{2}$ and $\mathbf{t}_{AB} = \frac{1}{2}\mathbf{t}_{AA} = \frac{1}{2}\mathbf{t}_{BB}$.

The theory can be extended in an obvious manner to the case of several motif points within the primitive unit cell.

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The Crystal Structure of 1,4-Dithiane*

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The crystal structure of 1,4-dithiane has been determined and refined by least-squares methods, using complete three-dimensional diffraction data from copper X-radiation. The compound is isomorphous with 1,4-diselenane, and hence the molecule has the centro-symmetric chair configuration, as reported by Dothie. The bond distances and standard deviations are: S–C_1, 1·801± 0·013 Å; S–C_2, 1·821±0·011 Å; C_1–C_2, 1·490±0·018 Å.

Introduction

In an electron-diffraction investigation of 1,4-dithiane, $C_4H_8S_2$, Hassel & Viervoll (1947) reported sulfur–carbon distances of approximately 1·81 Å, which is the sum of the accepted single-bond radii of carbon and sulfur (Pauling, 1948), but were unable to differentiate between two different models for the molecule. An X-ray diffraction investigation of 1,4-diselenane (Marsh & McCullough, 1951) showed that this molecule has the expected chair form; however, the average Se–C distance proved to be 2·01 Å—significantly greater than the sum of the single-bond radii of selenium and carbon (1·94 Å). The present X-ray diffraction investigation of crystals of 1,4-dithiane was undertaken to provide a check on the S–C distances, as well as to ascertain the molecular configuration. Recently, Dothie (1953) has reported unit-cell dimensions and space-group symmetry for 1,4-dithiane which require that the molecule be in the centro-symmetric chair configuration.

Experimental

A sample of 1,4-dithiane was recrystallized by slow sublimation in a sealed ampoule. The resulting monoclinic crystals, which were elongated in the *b* direction, were sealed in thin-wall glass capillaries to prevent evaporation during X-ray photography. Two crystals were photographed; one was oriented with its *b* axis parallel to the axis of the capillary and had dimensions of about 0·5×1·5×0·2 mm., while the other had its *c* axis approximately parallel to the axis of the capillary and had dimensions of about 0·3×0·4×0·2 mm. Multiple-film Weissenberg photographs were prepared with unfiltered copper X-radiation for the equator and first four layer lines about the *b* axis, and for the equator and first six layer lines about the *c* axis; by this means, all of the reflections within the sphere of copper radiation were recorded. Out of the total of 618 reflections within the sphere, 548 were strong enough to be observed. Intensities were estimated visually by comparison with a calibrated strip, and a film factor of $3{\cdot}8^{\sec\mu}$ was used to correlate intensities of successive photographs, μ being the equi-inclination angle. No correction was made for absorption.

The space-group symmetry, as determined from the Weissenberg photographs, is that of C_{2h}^5–$P2_1/n$. Approximate unit-cell dimensions and intensity comparisons showed that the compound is isomorphous with 1,4-diselenane (Marsh & McCullough, 1951); there are thus two centro-symmetric molecules in the unit cell, in agreement with the findings of Dothie (1953). Accurate values for the lattice parameters

Table 1. *Lattice parameters*

	1,4-Dithiane		
	This investigation (1)	Dothie (2)	1,4-Diselenane (3)
a	6·763±0·002 Å	6·74 Å	6·97±0·02 Å
b	5·464±0·005 Å	5·46 Å	5·62±0·02 Å
c	7·844±0·003 Å	7·69 Å	8·01±0·02 Å
β	92·67 ±0·04°	91·53°	93·6 ±0·1°
c'	10·12 ±0·008 Å	10·09 Å	—
β'	129·25 ±0·07°	130·37°	—

(λ = 1·5418 for Cu $K\alpha$, 1·54050 for Cu $K\alpha_1$, 1·54434 for Cu $K\alpha_2$)

* Contribution No. 1926 from The Gates and Crellin Laboratories of Chemistry.