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A Classification of Cylindrical Lattices

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There is evidence that certain minerals, particularly chrysotile, have cylindrical structures which possess a degree of order definable in terms of a cylindrical lattice. A classification and enumeration of the possible types of such lattices is made in order to clarify the possibilities of structural variation in such minerals. The possible symmetry properties of such structures are also discussed.

1. Introduction

It is now generally accepted on the evidence of electron microscopy (Bates, Sand & Mink, 1950; Noll & Kircher, 1951, 1952) that chrysotile, garnierite and halloysite have a tubular structure. Jagodzinski & Kunze (1954*a*, *b*, *c*) and Whittaker (1954, 1955*a*, *b*) have discussed the X-ray diffraction phenomena to be expected from a tubular structure in which the wall consists of a succession of equally spaced layers mutually ordered in the direction parallel to the cylinder axis, and these are in general agreement with the diffraction phenomena obtained from chrysotile.

It has been known for some years that chrysotile exists in two forms apparently based on orthorhombic and monoclinic lattices (Whittaker, 1952), and before the nature of the cylindrical-lattice structure was appreciated there were discussions as to whether the normal form had a triclinic or monoclinic unit cell (Padurow, 1950; Whittaker, 1951). More recently Jagodzinski & Kunze (1954*c*) have found evidence of a helical structure. It is therefore of interest to ascertain what structure types can be expected among structures of tubular form, and also to what extent the usual crystallographic concepts of projections and space groups can be applied to them.

2. Definition of a cylindrical lattice

A cylindrical lattice consists of a set of congruent two-dimensional lattices inscribed on a set of cylindrically curved surfaces and mutually ordered with respect to the cylinder axis, there being equal and uniform normal spacings between each successive pair of such surfaces.

We may define the following parameters of such a lattice:

a' is the normal spacing between each successive pair of cylindrical surfaces.

b and c are the lattice parameters of the two-dimensional lattice (the generating lattice); of these c is taken as that which is the more nearly parallel to the cylinder axis.

α is the angle included between the b and c axes.

β is an angle such that each successive two-dimensional lattice is displaced by a distance $a' \cot \beta$, parallel to the cylinder axis, with respect to its inner neighbour.

It will then be convenient to put $a = a' \operatorname{cosec} \beta$.

This definition would include lattices inscribed on any set of cylindrically curved surfaces whose right section constituted a set of equally spaced involutes of the same figure. Real structures, however, will be based only on those lattices which are free from loops and intersections, and we are here concerned primarily with those which are capable of forming a tubular structure. Moreover, it is to be expected that a curved layer free from external anisotropic constraints will conform only to a curve whose radius of curvature is constant or a monotonic function of arc length. We shall therefore consider in detail only those lattices whose right sections are sets of equally spaced circles, or the successive turns of the involute of a circle. The latter will be referred to as spiral lattices.

3. Possible types of circular cylindrical lattices

In a cylindrical lattice it is impossible that two axes should be symmetrically equivalent since they are all uniquely definable, and we shall therefore take no account of cylindrical lattices in which two or more of the axial parameters are equal in length. There exist, therefore, three main types, corresponding in their angular parameters to three of the crystal systems, as follows:

Anorthic: $\alpha \neq \beta \neq \frac{1}{2}\pi$ (the name anorthic is clearly preferable to triclinic since only two angles can be specified).

Monoclinic: two cases can be distinguished: $\beta \neq \alpha = \frac{1}{2}\pi$ and $\alpha \neq \beta = \frac{1}{2}\pi$.

Orthorhombic: $\alpha = \beta = \frac{1}{2}\pi$ (no rhomb can be defined, but the name will serve by analogy in the absence of the name aclinic).

It will first be assumed that the b axis lies in a right section of the cylinder. It then follows that there is a relation between a and b for such lattices which is necessary for their existence, namely

$$nb = 2\pi a',$$

where n is an integer. This ensures that there is an integral number of b units on every layer provided that there is an integral number on one layer. Subject to this condition the following lattice types may be defined:

(i) Anorthic of the 1st kind, $\alpha \neq \beta \neq \frac{1}{2}\pi$. This is generated by an oblique two-dimensional lattice, one axis of which is oriented perpendicular to the cylinder axis. Successive layers are displaced parallel to this axis by an amount $a' \cot \beta$.
(ii) Monoclinic of the 1st kind, $\beta \neq \alpha = \frac{1}{2}\pi$. This results if the generating lattice in (i) is made rectangular.
(iii) Monoclinic of the 2nd kind, $\alpha \neq \beta = \frac{1}{2}\pi$. This results from (i) if the displacements of the successive layers are set equal to zero.
(iv) Orthorhombic of the 1st kind, $\alpha = \beta = \frac{1}{2}\pi$. This results from (ii) if the displacements of the successive layers are set equal to zero, or from (iii) if the generating lattice is made rectangular.

For reasons which will appear later, these lattice types will be referred to as the regular series.

If the b axis is inclined to the right section of the cylinder then it must lie on a helix. This would arise, for example, if the rectangular lattice shown in Fig. 1

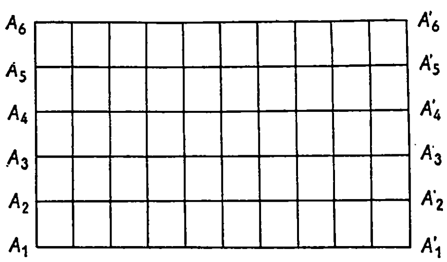

Fig. 1.

were wrapped into a cylinder so that A_1 is joined to A'_2, A_2 to A'_3 etc.; or in the general case so that A_n is joined to A'_{N+n}. Then if a set of such cylinders were stacked one within the other we might expect to obtain a second series of helical lattice types analogous to the above, i.e.

(v) Anorthic of the 2nd kind, $\alpha \neq \beta \neq \frac{1}{2}\pi$.
(vi) Monoclinic of the 3rd kind, $\beta \neq \alpha = \frac{1}{2}\pi$.
(vii) Monoclinic of the 4th kind, $\alpha \neq \beta = \frac{1}{2}\pi$.
(viii) Orthorhombic of the 2nd kind, $\alpha = \beta = \frac{1}{2}\pi$.

Types (v)–(viii) may indeed occur in real structures, but the following argument shows that they cannot be geometrically perfect. Consider the most general case, an anorthic lattice of the 2nd kind, in which the innermost cylinder has a radius a_0 and the b axis on the layer of radius (a_0+ma') makes an angle δ_m with a right section. Then for ordered stacking of the layers to be possible in the direction of the cylinder axis it is necessary that the pitch of the b-axis helix should be the same on every layer. Let this pitch be t. Then δ_m may be defined by the relation

$$\tan \delta_m = \frac{Nt}{2\pi(a_0+ma')}. \tag{1}$$

But

$$c = \frac{t \cos \delta_m}{\sin \alpha}. \tag{2}$$

Hence at least one of the parameters c and α must vary from layer to layer to satisfy (2). Also, if p_m is the number of b units in the developed form of the generating lattice, then

$$\begin{aligned} p_m &= \frac{2\pi(a_0+ma') \sin(\alpha+\delta_m)}{b \sin \alpha} \\ &\simeq \frac{2\pi(a_0+ma')}{b}\left(1+\frac{Nt \cot \alpha}{2\pi(a_0+ma')}-\frac{N^2t^2}{8\pi^2(a_0+ma')^2}\right). \end{aligned} \tag{3}$$

It follows that if p_m is integral at least one further parameter of the set a, b and α must vary with m, or alternatively that local imperfections occur associated with non-integral values of p_m.

The distortions required to satisfy relations (2) and (3) may, however, be very small. In chrysotile, for example, where $\alpha = \frac{1}{2}\pi$, the total strain in any layer would not exceed 0·05% for $n = 1$, even if a_0 were assumed to be as small as 30 Å; and since chrysotile has a centred lattice (see § 7) half integral values of N are permitted, so that a helical lattice with a maximum strain of only one-quarter of this is possible. Such lattices may therefore be of practical importance.

4. Possible types of spiral cylindrical lattice

As before, we assume first that the b axis lies on a right section of the cylinder. It then follows that $\beta = \frac{1}{2}\pi$, since the successive turns of the spiral formed by the b axis of the generating lattice are coplanar. There are, therefore, only two possible regular lattice types in these circumstances, which may be named as follows in conformity with the nomenclature introduced for the circular cylindrical lattices:

(i) Monoclinic of the 2nd kind, $\alpha \neq \beta = \frac{1}{2}\pi$.
(ii) Orthorhombic of the 1st kind, $\alpha = \beta = \frac{1}{2}\pi$.

The anorthic lattice of the 1st kind and the monoclinic lattice of the 1st kind cannot exist. No relationship between the lattice parameters is imposed by the construction of a spiral cylindrical lattice.

If the b axis does not lie on a right section of the cylinder then it follows that $\beta \neq \frac{1}{2}\pi$. Therefore a monoclinic lattice of the 4th kind and an orthorhombic lattice of the 2nd kind cannot exist. Moreover, the remaining lattice types cannot exist in a geometrically perfect form, for the b axis must advance a distance $a' \cot \beta$ along the cylinder axis for every turn of the spiral. It must therefore be inclined to the right section of the cylinder at any given point of the cylinder at an angle given by $\sin \delta = a' \cot \beta / 2\pi\varrho$, where ϱ is the radius of curvature of the cylinder at that point. This clearly varies continuously along the b axis, so that either the axes of the generating lattice must be curved, or the angle β must vary throughout the lattice. However, the distortions involved may once again be very small in practical cases. For example, in chrysotile the maximum curvature required in the generating lattice would involve a total change of direction throughout the lattice of about 10′, although the corresponding variation in β if the b axis of the generating lattice were straight would be of the order of 5°.

In view of these considerations it appears that the necessarily slightly imperfect helical spiral cylindrical lattices of the following types may also be of practical interest:

(iii) Anorthic of the 2nd kind, $\alpha \neq \beta \neq \frac{1}{2}\pi$.
(iv) Monoclinic of the 3rd kind, $\beta \neq \alpha = \frac{1}{2}\pi$.

5. Incomplete cylindrical lattices

If a cylindrical lattice subtends an angle less than 2π at all points of the cylinder axis, then all the restrictions on the existence of the various lattice types disappear, and the imperfections in the helical series due to relation (3) disappear, but those due to relation (2) remain.

6. Relationships of the cylindrical-lattice types

The relation between the various possible circular and spiral cylindrical-lattice types is clarified by Table 1. The letters R and H denote the existence of a lattice of the specified type in the regular or the helical series respectively.

7. Centred cylindrical lattices

The analogy between the theory of cylindrical lattices and normal crystallographic theory may be carried further if the concept of centred lattices is introduced.

In cylindrical lattices which have a rectangular generating lattice (all those with $\alpha = \frac{1}{2}\pi$) the latter may be either primitive (p) or centred (a).

A second type of lattice analogous to a centred lattice arises if one or more sets of similar cylindrical lattice layers are intercalated between those which define the repeating unit in the radial direction. Such intercalated sets of layers will constitute co-axial cylindrical lattices having the same parameters a, b, c, α and β, but having different values of a_0 and relative displacements parallel to the cylinder axis. Such composite lattices may be denoted by c_n, if the intercalated layers divide the a' spacing into n equal parts.

8. Cylindrical projections

Up to this point only the geometrical arrangement of lattice points has been considered. In real structures, however, there will be a distribution of matter associated with each lattice point. Such a distribution of matter cannot conform to a three-dimensional space group, since there is no unit of the structure which repeats regularly in three dimensions. It is possible, however, to define two projections of such a distribution which will constitute regular two-dimensional repeating patterns whose symmetry can be discussed in terms of two-dimensional space groups.

It is evident that a cylindrical structure of the kind under discussion can only be formed by a layer structure, the individual layers of which have dissimilar sides, and the successive layers of which have negligible steric interactions with one another in the b-axis direction. It follows that in such a structure these layers constitute zones lying between parallel circular or spiral cylindrical surfaces within which the structure is coherent. If any intensive property of the structure (e.g. electron density) is integrated along the normals to these surfaces over the thickness of the layer and projected on to the neutral surface of the layer with respect to bending, then the two-dimensional projection so obtained will form a regular repeating pattern. It may conveniently be described as the cylindrical projection on (100) by analogy with normal crystallographic nomenclature. This projection is based on the generating lattice of the structure, and is identical for every layer of the structure, although the different layers themselves differ from one another in detail as a result of their different curvatures.

Table 1

	Kind	Inter-axial angles	Orientation of b axis to right section	Circular	Spiral
Anorthic	1st	$\alpha \neq \beta \neq \frac{1}{2}\pi$	Parallel	R	—
	2nd		Inclined	H	H
Monoclinic	1st	$\beta \neq \alpha = \frac{1}{2}\pi$	Parallel	R	—
	2nd	$\alpha \neq \beta = \frac{1}{2}\pi$	Parallel	R	R
	3rd	$\beta \neq \alpha = \frac{1}{2}\pi$	Inclined	H	H
	4th	$\alpha \neq \beta = \frac{1}{2}\pi$	Inclined	H	—
Orthorhombic	1st	$\alpha = \beta = \frac{1}{2}\pi$	Parallel	R	R
	2nd		Inclined	H	—

A second regular projection may be defined as follows. Take any plane orthogonal to the cylindrical surfaces of the lattice. From every point on this plane construct an arc parallel to the b axis of the lattice which lies within the same layer. Continue each arc until a point is reached whose environment in the cylindrical surface on which it lies is identical with that at the starting point of the arc. If any intensive property of the structure is summed and projected along the arc on to the initial plane then a regular two-dimensional repeating pattern is obtained. This pattern lies on a lattice with parameters a, $c \sin (\alpha+\delta_m)$, and included angle β. It may conveniently be described as the cylindrical projection down [010]. It has previously been shown (Whittaker, 1954) that the amplitudes of the $h0l$ reflexions from a structure based on orthorhombic or monoclinic lattices of the 1st kind are proportional to the Fourier components of the electron-density projection defined in this way.

9. Symmetry in cylindrical projections

The cylindrical projection on (100) may have any of the two-dimensional space groups belonging to the oblique and rectangular systems. But, because the inside and outside of a layer must be dissimilar, it is not permissible for the cylindrical projection down [010] to contain either a twofold rotation point or a symmetry line perpendicular to the a axis. Therefore the only permissible two-dimensional space groups in this projection are $p1$, pm, pg, and cm, in the usual notation, and their orientations are subject to restrictions. In order to make these restrictions clear it is convenient to use full space-group symbols with the same conventions as to order of the symbols as in the three-dimensional orthorhombic space groups, and to use a and b to denote centred lattices on the projections on (100) and down [010] respectively. The notation of the possible space groups in the latter projection is then $p11$, $p11m$, $p11g$, and $b11m$. The alternative orientations $pm11$, $pg11$, and $bm11$ are not permitted.

10. Cylindrical lattices and dislocations

Jagodzinski & Kunze (1954c) have already pointed out that spiral and helical cylindrical structures may be described in terms of radial and axial dislocations. It is in fact possible to give a formal description of all the cylindrical lattices discussed above in terms of dislocations introduced into a normal three-dimensional lattice of appropriate dimensions.

Thus a regular circular cylindrical lattice may be considered to arise by the introduction of regularly spaced edge dislocations of Burgers vector $\mathbf{b}$ parallel to the cylinder axis, with a density of $a'/b\varrho$ in the layer of radius ϱ. Such a lattice may then be converted to a regular spiral by introduction of a Volterra edge dislocation along the axis with Burgers vector $\mathbf{a}'$, and a regular lattice may be converted to a helical one by a Volterra screw dislocation along the axis with Burgers vector $N\mathbf{t}$. However, these descriptions are purely formal. It is not to be supposed that the lattice is stressed in the usual way by these dislocations; rather it is the unstressed shape of the structural elements that leads to the configurations described, and therefore the concept of a cylindrical lattice is preferable to that of a dislocated normal three-dimensional lattice which has no real existence.

In addition to these formal considerations, we may envisage that dislocations with their normal significance may be introduced into cylindrical lattices. The following cases are worthy of note, although no evidence is available at present for their existence or stability.

(i) A radial screw dislocation would involve a join between a circular and a spiral cylindrical lattice.
(ii) A screw dislocation parallel to the axis but not along it would introduce a measure of helical structure in a regular cylindrical lattice without converting it into a helical lattice, and would thus provide a longitudinal growth mechanism for a regular cylindrical lattice.
(iii) Radial edge dislocations with Burgers vector $\mathbf{b}$ could convert cylindrical lattices into tapering or conical structures.

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