relative to the local lattice vector. It then gives a measure of the crystal-grain size or the distance between points in the crystal that scatter the X-rays.

It is likely that the major influence on this model is the kinematic assumption, which will fail for thicker films when the extinction of the transmitted beam is important. This means that the reflectance becomes large and the quadratic term in (1) cannot be neglected. In such instances, dynamical models (Kato, 1980; Becker & Al Haddad, 1990; Davis, 1991) must be used.

Concluding remarks

A stochastic model for crystal defects has been developed that leads to a correlation function that is used to calculate the reflectivity of imperfect crystals containing defect planes and crystal grains. A solution for the kinematical reflectivity has been given involving a convolution between the perfect-crystal reflectivity and a function depending on two parameters related to the crystal defects. This function takes the limiting form of a Gaussian or a Lorentzian function depending on a correlation length. In a subsequent paper, the fit of this kinematic solution to experimental data will be discussed. The defect model has been incorporated previously in a model for dynamical X-ray diffraction that leads to a partial differential equation for a probability density describing the crystal reflectance (Davis, 1991).

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Cubic Cylinder Packings

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Abstract

Five basic cubic packings of symmetry-related cylinders are described. Four are stable packings and two were described by O'Keeffe & Andersson [*Acta Cryst.* (1977). **A33**, 914-923]. The possible symmetries of rods that can replace the cylinders in crystal structures are identified. Replacing cylinders by bundles of cylinders produces a total of 23 cubic cylinder packings, of which 18 are stable.

Introduction

The study of packings of objects such as spheres or polyhedra (representing atoms or groups of atoms) has played an essential role in descriptive crystal chemistry for a long time. More recently, packings of cylinders (representing rods of atoms) have been used similarly. Some cylinder packings and their applications to crystal chemistry were described by O'Keeffe & Andersson (1977) - hereinafter OKA - who described eight packings. The term cylinder packing is used here to refer to infinite packings of cylinders in which every cylinder is related to all the others by crystallographic symmetry operations. Two cubic packings were found to be particularly useful in descriptive crystal chemistry when the cylinders were replaced by rods of atoms. These packings were referred to as 'body-centered cubic rod packing' and

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'primitive cubic rod packing'; here they are named after structures in which they are a particularly conspicuous feature, namely garnet (Andersson & O'Keeffe, 1977) and β-W, respectively. In the garnet packing the rod axes lie on four nonintersecting threefold symmetry axes; in the β-W packing the rod axes lie on three nonintersecting fourfold symmetry axes.

The cubic β-manganese structure (Shoemaker, Shoemaker, Hopkins & Yindepit, 1978) was described by OKA as a garnet packing of rods of metaprisms and tetrahedra aligned along the four nonintersecting threefold axes of $P4_132$. Recently, Nyman, Carroll & Hyde (1991) have shown that a particularly appealing alternative description of the same structure is as a packing of rods of face-sharing tetrahedra packed with rod axes along nonintersecting 4_1 axes. In both instances all the atoms in the crystal lie on the corresponding rods. The cylinder packing corresponding to the rod packing in the description of Nyman *et al.* (1991) was not in the compilation of OKA and is described here together with two new cubic packings with cylinders on four nonintersecting $3_{1,2}$ axes.

The location of cylinder axes is most readily specified as the line of intersection of two planes. The line of intersection of planes $x = x_0, y = y_0$ is written as x_0, y_0, u where u can take any value. Likewise, $\frac{1}{3}+u, \frac{2}{3}+u, u$ indicates the line of intersection of $x = z+\frac{1}{3}$ and $y = z+\frac{2}{3}$.

In deriving crystal structures the cylinders must be replaced by rods of atoms and it is useful to know the rod symmetries. These are given using conventional crystallographic symbols (Shubnikov & Koptsik, 1974) with **p** representing the one-dimensional lattice with translations along **c**. The reader unfamiliar with rod-symmetry groups can find a good introduction in Smith (1982).

The β-Mn cylinder packing

The packing of cylinders corresponding to the description by Nyman *et al.* (1991) of the β-Mn structure is succinctly described as: space group $I4_132$, cylinder axes $\frac{1}{4}, 0, u$; $\frac{3}{4}, \frac{1}{2}, u$; $u, \frac{1}{4}, 0$; $u, \frac{3}{4}, \frac{1}{2}$; $0, u, \frac{1}{4}$; $\frac{1}{2}, u, \frac{3}{4}$. These are derived from the general positions $48(i)$ of $I4_132$ by the substitution $x = \frac{1}{4}, y = 0, z = u$. For cylinders of unit diameter the cell edge is $a = 4$. This structure is called β-Mn. The maximum symmetry of rods aligned with the cylinder axes is $\mathbf{p}4_122$. The substitution $\frac{3}{4}, 0, u$ results in rod symmetry $\mathbf{p}4_322$ (note that $I4_132$ has both 4_1 and 4_3 axes).

The new structure is simply derived by removing one-half of the cylinders of the β-W packing. A sketch of these structures is shown in Fig. 1 in which the $Pm\bar{3}n$ packing is described using a doubled cell and an origin appropriate for $Ia\bar{3}d$ (as discussed further below).

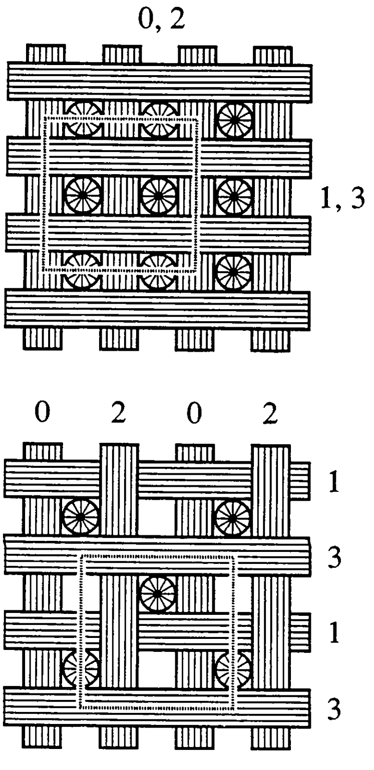


Fig. 1. Top: the β-W cylinder packing projected on (001). A doubled cell ($Ia\bar{3}d$) is outlined. Bottom: the β-Mn cylinder packing projected on (001). A unit cell ($I4_132$) is outlined. Numbers are the elevations of cylinder axes in units of $a/4$.

The SrSi$_2$ cylinder packing

In the structure of SrSi$_2$ (Janson, Schäfer & Weiss, 1965), the Si atoms are in positions $8(c)$ of $P4_132$ x, x, x, with $x = 0.17$. If $x = 0.125$ one has the invariant-lattice complex (Fischer & Koch, 1983) $^+Y^*$ corresponding to positions $8(a)$ of $I4_132$ and for convenience this slightly idealized description is used here. The Si atoms form 3_1 helices parallel to ⟨111⟩. The axes of the helices are derived from the general positions of $I4_132$ by the substitution $x = \frac{1}{3}+u, y = \frac{2}{3}+u, z = u$. These axes also correspond to the axes of a cylinder packing that is derived from garnet by removal of eight out of every nine cylinders. For unit-diameter cylinders, the cell edge is $6\times 2^{1/2}$. The cylinder axes are $\frac{1}{3}+u, \frac{2}{3}+u, u$; $\frac{1}{6}+u, \frac{2}{3}-u, u$; $\frac{2}{3}+u, \frac{5}{6}+u, -u$; $\frac{5}{6}-u, \frac{5}{6}+u, u$. The enantiomorphic structure with 3_2 axes is obtained by the substitution $\frac{2}{3}+u, \frac{1}{3}+u, u$ in the general positions. The structure is shown in projection in Fig. 2 and a model is displayed in Fig. 3(a).

The γ-Si cylinder packing

In the structure of γ-Si (Kasper & Richards, 1964) with symmetry $Ia\bar{3}$, four-coordinated Si atoms are in $16(c)$ x, x, x, with $x = 0.100$. All the atoms fall on ⟨111⟩

strings arranged in a garnet packing. This description suggests a simple relationship to a b.c.c. lattice as follows. The set $16(c)$ of $Ia\bar{3}$ splits into two sets $8(a)$ (again x, x, x) of $I2_13$ with $x_1 = 0.100$ and $x_2 = 0.400$. If these parameters are changed to $x_1 = 0.0$ and $x_2 = 0.25$, the structure is that of the b.c.c. lattice.

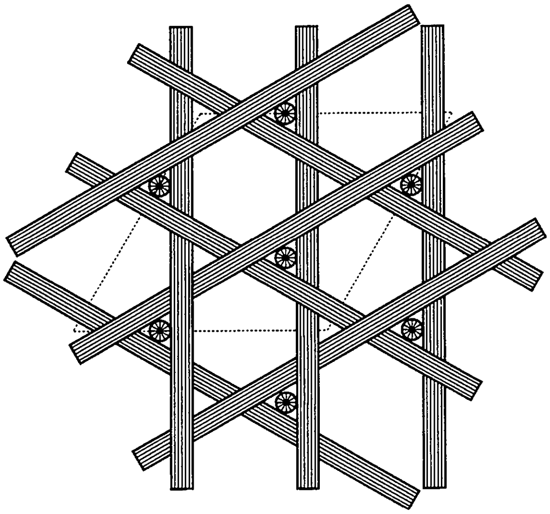
An alternative description of the γ-Si structure (von Schnering & Nesper, 1987) focuses on 3_1 and 3_2 helices of Si atoms again parallel to $\langle 111\rangle$. If the x parameter of $16(a)$ of $Ia\bar{3}$ is changed from 0.1 to 0.125 the structure will have symmetry $Ia\bar{3}d$ and the positions correspond to the invariant lattice complex Y^{**}, *i.e.* an intergrowth of ${}^+Y^*$ and ${}^-Y^*$. The axes of these helices therefore represent an intergrowth of the two enantiomorphic $SrSi_2$ cylinder packings and is derived from the garnet packing by removal of seven out of every nine cylinders. This structure is called the γ-Si packing. It is not a stable cylinder packing because cylinders of one set are not in contact with cylinders of the other set, so that one set can move with respect to the other. The two sets of cylinders are separated by the periodic minimal surface Y^{**} [*cf.* Fig. 6(a) of von Schnering & Nesper (1987)]. A model displaying the two sets of cylinders is shown in Fig. 3(b).

The most symmetrical form of the packing has symmetry $Ia\bar{3}d$ and the cylinder axes are obtained by the substitution $\frac{2}{3}+u, \frac{1}{3}+u, u$ for x, y, z in the general positions. For unit-diameter cylinders the cell edge is $6\times 2^{1/2}$.

Rod packings and symmetry

The fact that two complementary descriptions of the β-manganese structure were possible reflects the fact that cubic space groups that have nonintersecting threefold axes also have symmetry-related sets of nonintersecting two- or fourfold axes along $\langle 001\rangle$ that also do not intersect the threefold axes. Thus in $Ia\bar{3}d$, positions $32(e)$, expressed as u, u, u *etc.*, correspond to the axes of cylinders parallel to $\langle 111\rangle$ and positions $48(f)$, expressed as $0, \frac{1}{4}, u$ *etc.*, correspond to cylinder axes parallel to $\langle 001\rangle$. One can therefore interweave the two cylinder packings. In particular, the description by OKA of the garnet structure (of *e.g.* $Ca_3Al_2Si_3O_{12}$) as a $\langle 111\rangle$ packing (along u, u, u *etc.*) of nonintersecting rods of AlO_6 octahedra alternating with (face-sharing) empty O_6 trigonal prisms can be supplemented by observing that the remaining atoms are nonintersecting $\langle 001\rangle$ strings of alternating Si and Ca atoms (along $0, \frac{1}{4}, u$ *etc.*) thereby accounting for all the atoms in the structure in a particularly satisfying manner.

When cylinders of a packing are replaced by rods, the symmetry of the resulting structure may be reduced. In Table 1, the possible cubic space groups for rod packings and the corresponding rod symmetries are listed. This table should prove useful for identifying rod packings in crystal structures and for inventing possible new crystal structures.



F. ;. 2. A fragment of the $SrSi_2$ cylinder packing projected on (111). A hexagonal unit cell is outlined.

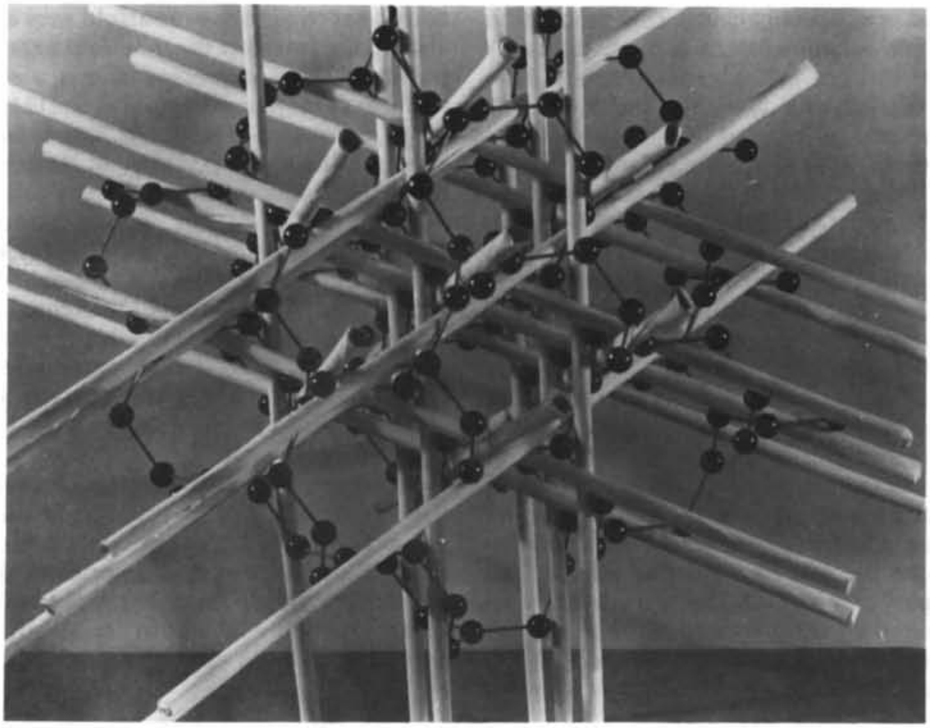
Packings of bundles of cylinders

Other cubic cylinder packings can be derived by replacing cylinders of the five packings described so far by bundles of cylinders. This is somewhat analogous to the process of obtaining rare sphere packings from denser ones by replacing spheres by groups of spheres (O'Keeffe, 1991). OKA illustrated the procedure in deriving their structure (vii) from (vi).

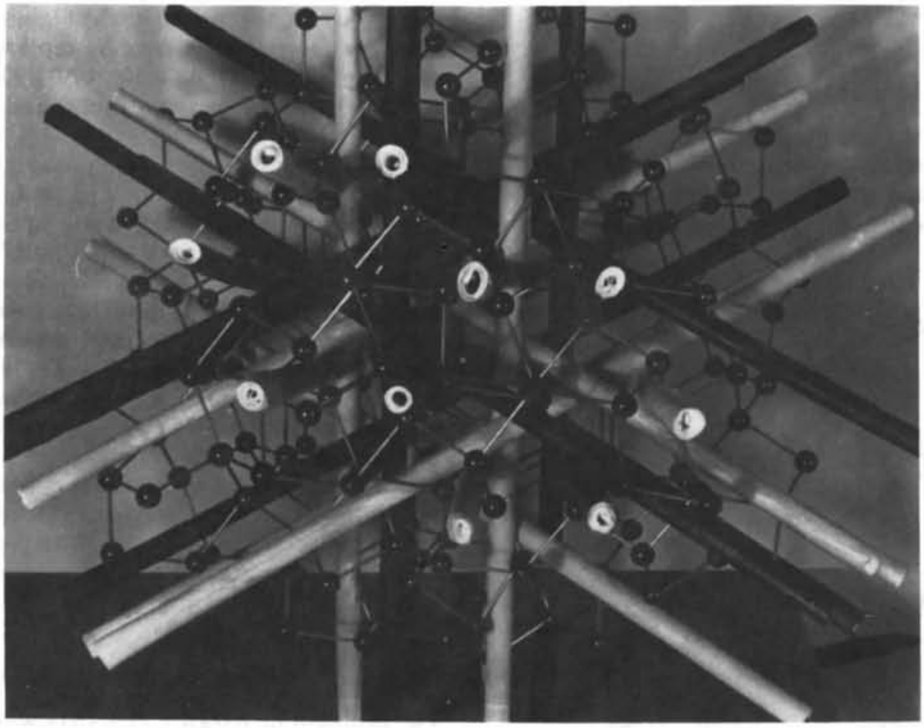
Possible bundles for stable packings of equivalent cylinders are illustrated in Fig. 4. In the β-W and β-Mn structures, the rods fit into square tunnels and have projection symmetry $4mm$; possible bundles for stable packings are $S1$, $S2$, $S4_1$, $S4_2$ and $S8$. In the $SrSi_2$ packing, rods fit into triangular tunnels and have projection symmetry $3m$; possible bundles for stable packings are $T1$, $T3_1$, $T3_2$ and $T6$. These bundles are also possible substitutions in the intergrowth structure γ-Si. In the garnet structure the rods fit into hexagonal tunnels and have projection symmetry $6mm$; stable possibilities are $H1$, $H3$, $H6_1$, $H6_2$ and $H12$. In this way one can generate 15 new cylinder packings and 3 new intergrowth packings. These are summarized and their densities given in Table 2.

Density of cylinder packings

The problem of packing cylinders with parallel axes is the same as that of packing circles on a plane and the same fraction of space (the density) is covered. The density (O'Keeffe & Hyde, 1980) will range from $3^{1/2}\pi/(7+4\times 3^{1/2}) = 0.3907$ for cylinder axes on a



(*a*)



(*b*)

Fig. 3. (*a*) A model of the $SrSi_2$ cylinder packing in a framework of a ball-and-spoke model of positions 8(*a*) of $I4_132$. (*b*) A model of the γ-Si intergrowth cylinder packing in a framework of a ball-and-spoke model of the γ-Si structure.

Table 1. *Occurrence of cylinder-packing axes in the cubic space groups and the associated rod symmetries*

In the table, the headings are the structures and the location of axes using the origins chosen in *International Tables for Crystallography* (1983). The individual entries are the generated Wyckoff positions and the rod symmetries of the axes. In the symbols for the rod-symmetry groups, **p** refers to the one-dimensional lattice and the translation direction is parallel to **c**.

Symmetry group	Garnet	γ-Si	β-W (×2)	
	u, u, u	$\frac{1}{3}+u, \frac{2}{3}+u, u$	$0, \frac{1}{4}, u$	$\frac{1}{4}, 0, u$
$Ia\bar{3}d$	e, $\mathbf{p}\bar{3}c1$	h, $\mathbf{p}3_12, \mathbf{p}3_22$	f, $\mathbf{p}\bar{4}c2$	h, $\mathbf{p}4_122, \mathbf{p}4_322$
$I\bar{4}3d$	c, $\mathbf{p}3c1$	e, $\mathbf{p}3_1, \mathbf{p}3_2$	d, $\mathbf{p}\bar{4}$	e, $\mathbf{p}222_1$
$Ia\bar{3}$	c, $\mathbf{p}\bar{3}$	e, $\mathbf{p}3_1, \mathbf{p}3_2$	d, $\mathbf{p}cc2$	e, $\mathbf{p}222_1$
$Pa\bar{3}$	c, $\mathbf{p}\bar{3}$	d, $\mathbf{p}3_1, \mathbf{p}3_2$	d, $\mathbf{p}1c1$	d, $\mathbf{p}112_1$

Symmetry group	Garnet	SrSi$_2$		β-W (×2)	β-Mn	
	u, u, u	$\frac{1}{3}+u, \frac{2}{3}+u, u$	$\frac{2}{3}+u, \frac{1}{3}+u, u$	$0, \frac{1}{4}, u$	$\frac{1}{4}, 0, u$	$\frac{3}{4}, 0, u$
$I4_132$	e, $\mathbf{p}3$	i, $\mathbf{p}3_12$	i, $\mathbf{p}3_22$	f, $\mathbf{p}222$	i, $\mathbf{p}4_122$	i, $\mathbf{p}4_322$
$P4_132$	c, $\mathbf{p}3$	e, $\mathbf{p}3_22$	e, $\mathbf{p}3_12$	e, $\mathbf{p}211$	e, $\mathbf{p}4_1$	e, $\mathbf{p}222_1$
$P4_332$	c, $\mathbf{p}3$	e, $\mathbf{p}3_22$	e, $\mathbf{p}3_12$	e, $\mathbf{p}211$	e, $\mathbf{p}222_1$	e, $\mathbf{p}4_3$
$I2_13$	a, $\mathbf{p}3$	c, $\mathbf{p}3_1$	c, $\mathbf{p}3_2$	b, $\mathbf{p}112$	c, $\mathbf{p}222_1$	c, $\mathbf{p}222_1$
$P2_13$	a, $\mathbf{p}3$	b, $\mathbf{p}3_2$	b, $\mathbf{p}3_1$	(b, $\mathbf{p}1$)	b, $\mathbf{p}112_1$	b, $\mathbf{p}112_1$

Symmetry group	β-W ($0, \frac{1}{2}$, u or $\frac{1}{2}, 0, u$)
$Pm\bar{3}n$	g or h, $\mathbf{p}4_2/mmc$
$P\bar{4}3n$	h or g, $\mathbf{p}\bar{4}2c$
$P4_232$	i or j, $\mathbf{p}4_222$
$Pm\bar{3}$	f or g, $\mathbf{p}mmm$
$P23$	g or h, $\mathbf{p}222$

3.12^2 net (the rarest such packing) to $\pi/12^{1/2} = 0.9069$ for cylinder axes on a 3^6 net (the densest cylinder packing). The packings based on the three regular and eight Archimedean tessellations exhaust the possibilities for packings with parallel axes.

The three basic cylinder packings with axes in parallel planes described by OKA all have the same density, $\pi/4 = 0.7854$. The cylinders of these packings can be replaced by bundles in limited and fairly obvious ways that are not further discussed here.

Densities of the cubic cylinder packings are recorded in Table 2. The garnet packing has density $3^{1/2}\pi/8 = 0.6802$ and SrSi$_2$ one-ninth of that. The β-W packing has density $3\pi/16 = 0.5890$ and the β-Mn packing one-half of that. The least dense stable packing of equivalent cylinders is conjectured to be the SrSi$_2$ packing of $T3_2$ bundles in which the fraction of space filled is only $3^{1/2}\pi/(56+32\times 3^{1/2}) = 0.04883$.

Table 2. *Densities of cubic cylinder packings*

The density is the fraction of space filled by cylinders. The cylinder bundles are identified in Fig. 4.

Structure	$S1$	$S2$	$S4_1$	$S4_2$	$S8$
β-W	0.5890	0.4043	0.5890	0.4043	0.4043
β-Mn	0.2945	0.2021	0.2945	0.2021	0.2021
Structure	$T1$	$T3_1$	$T3_2$	$T6$	
CaSi$_2$	0.0756	0.0911	0.0488	0.0608	
γ-Si	0.1511	0.1823	0.0977	0.1215	
Structure	$H1$	$H3$	$H6_1$	$H6_2$	$H12$
Garnet	0.6802	0.3645	0.5468	0.4534	0.3645

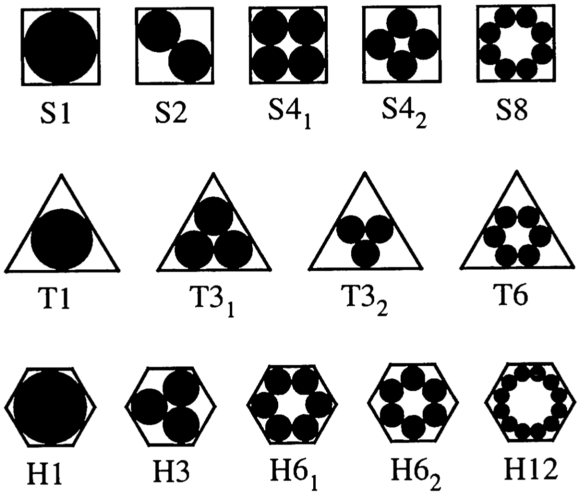


Fig. 4. Cross sections of the bundles of cylinders discussed in the text.

Concluding remarks

With hindsight, the basic cubic cylinder packings described here should have been 'obvious' as they simply represent the location of fourfold and threefold symmetry axes in certain cubic space groups (*International Tables for Crystallography*, 1983). They were found the hard way, by looking at crystal structures, and they have been found to be of great value for describing such structures (see, for example, OKA, Nyman *et al.*, 1991). Some at least have been illustrated in other contexts; an elegant model of the β-W packing using 432 cylinders has been constructed by Volten (1968) and a packing of right-triangular prisms with the $SrSi_2$ structure has been illustrated by Holden (1971). There is evidence that the $SrSi_2$ and β-Mn packings serve as the basis of the cubic structures observed in the 'blue phases' of cholesteric liquid crystals (Meiboom, Sammon & Berremann, 1983, and references therein).

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Decagrammal Symmetry of Decagonal $Al_{78}Mn_{22}$ Quasicrystal

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Abstract

General ideas about symmetries of quasicrystals based on simple self-similar tiling models and their mathematical formulation in terms of higher-dimensional multimetrical space groups find extensive confirmation in the structure of the decagonal $Al_{78}Mn_{22}$ quasicrystal phase. There is an incredible richness and variety of symmetries involving, in addition to mirror, rotation, translation and screw-rotation symmetries, planar and linear scalings as well, together with involutions generating those scalings, with and without associated nonprimitive translations. The linear parts of these symmetries generate a point group of infinite order, not yet fully investigated but, up to now, consistent with the symmetry of a self-similar decagram. The applicability of these symmetries to the atomic structure of the quasicrystal $Al_{78}Mn_{22}$ observed in nature requires the concept of higher-dimensional crystal forms and their projections in the physical space and in the internal space, respectively.

1. Introduction

One of the most striking characteristics of the diffraction pattern of many quasicrystals is the (discrete) scaling invariance of the positions of the Bragg peaks (Kuriyama & Long, 1986; Long & Kuriyama, 1986; Ostlund & Wright, 1986). That property is also found in simple classical models of quasicrystal structures described in terms of aperiodic tilings. Examples are, in one dimension, the Fibonacci and the octagonal chains and, in two and three dimensions, the Penrose tiling. The scaling property of the diffraction pattern is a consequence of the fact that those tilings are invariant with respect to appropriate inflation/deflation transformations. This means that, by combining inflation (deflation) with a rescaling of the distances, one gets the original pattern back.

The aim of the present paper is to demonstrate that scaling invariance can occur in quasicrystal structures, when described in terms of atomic positions. That will be shown by means of the concrete example of the decagonal $Al_{78}Mn_{22}$ quasicrystal phase on

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