Acta Crystallographica Section A
Foundations of Crystallography
ISSN 0108-7673

Received 1 August 2000
Accepted 24 August 2000

The invariant cubic rod (cylinder) packings: symmetries and coordinates

M. O'Keeffe,[a]* J. Plévert,[a] Y. Teshima,[b] Y. Watanabe[b] and T. Ogama[b]

[a]Materials Design and Discovery Group, Department of Chemistry, Arizona State University, Tempe, AZ 85287, USA, and [b]Institute of Applied Physics, University of Tsukuba, Tsukuba 305, Japan. Correspondence e-mail: mokeeffe@asu.edu

Six packings of symmetry-related cylinders, with cylinder axes in invariant positions (coordinates completely determined by symmetry), are described. Two have axes along ⟨100⟩ and four have axes along ⟨111⟩. It is shown that there can be no cubic cylinder packing with axes along ⟨110⟩. Earlier errors concerning the numbers of such packings and their symmetries are corrected.

1. Cubic cylinder packings

A number of recent papers (*e.g.* Duneau & Audier, 1999; Audier & Duneau, 2000) attest to the continued interest in periodic or quasi-periodic infinite packings of one-dimensionally infinite objects variously called rods, fibres or cylinders. Early work by O'Keeffe & Andersson (1977) on 'rod packings and crystal chemistry' was extended by O'Keeffe (1992) to a description of a number of homogeneous (*i.e.* all related by symmetry) 'cubic cylinder packings'; Ogawa *et al.* (1996) described various 'self-supporting rod structures' including some with cubic symmetry; and Parkhouse & Kelly (1998) discussed the 'regular packing of fibres', again including those with cubic symmetry. Despite their disparate titles, these last four works deal with the same topic, but they disagree in some respects on the number and descriptions of cubic packings, and this communication is to correct some of the earlier errors.

We are concerned with packings of non-intersecting rods (cylinders) with cubic symmetry; in particular, those corresponding to invariant line positions of the cubic space groups. In work to be published, we have enumerated these positions and can readily identify those corresponding to non-intersecting lines; they correspond to the positions of a certain set of symmetry axes of the space group. By analogy with the notation established (Fischer *et al.*, 1973; Fischer & Koch, 1983) for the invariant lattice complexes (point positions) we use Greek capital letters for the invariant line sets, with enantiomorphic pairs identified by prefixed + or − and intergrowth by a suffixed *. There are three cases to consider:

(*a*) *Lines (rod axes) along ⟨100⟩*. There are two sets: (i) Π^*: $\frac{1}{2}, 0, u$; $u, \frac{1}{2}, 0$; $0, u, \frac{1}{2}$ with symmetry $Pm\bar{3}n$, and (ii) $^{+}\Pi$: $\frac{1}{4}, 0, u$; $\frac{3}{4}, \frac{1}{2}, u$; $u, \frac{1}{4}, 0$; $u, \frac{3}{4}, \frac{1}{2}$; $0, u, \frac{1}{4}$; $\frac{1}{2}, u, \frac{3}{4}$ with symmetry $I4_132$. Both these structures are described by O'Keeffe (1992) who named them for the structures of β-W and β-Mn, respectively. The second structure is enantiomorphic and the rod symmetry of the axes of the structure given is $\mathbf{p}4_122$. The structure with rod symmetry $\mathbf{p}4_322$ is $^{-}\Pi$, and has coordinates $\frac{3}{4}, 0, u$ *etc*. The symbols for rod symmetries are explained in, for example, O'Keeffe & Hyde (1996). Interpenetration of the two enantiomorphs produces the first structure, *i.e.* $^{+}\Pi + {}^{-}\Pi = \Pi^*$. These structures are illustrated in Fig. 1.

(*b*) *Rod axes along ⟨110⟩*. O'Keeffe & Andersson (1977) and O'Keeffe (1992) do not discuss this case. Ogawa *et al.* (1996) found six cases of the same density and one of double density, but remarked that they are all uniaxial (*i.e.* not cubic). They are described in more detail by Ogawa *et al.* (1995). On the other hand, Parkhouse & Kelly (1998) discuss one such packing which they state is 'face-centred cubic' but they do not give the space group.

In fact it is easy to demonstrate that there can be no cubic packing of non-intersecting rods with axes along ⟨110⟩. Without loss of generality, we take an origin on a cubic threefold axis parallel to [111] (all origins for all cubic space groups are taken this way in *International Tables for Crystallography*). Consider the line $x_0 + u_1, y_0 - u_1, z_0$ passing through x_0, y_0, z_0 and parallel to $[1\bar{1}0]$. Rotation by one-third of a circle about the threefold axis mentioned will produce the line $z_0, x_0 + u_2, y_0 - u_2$ passing through z_0, x_0, y_0 and parallel to $[01\bar{1}]$. These two lines intersect at $z_0, x_0 + y_0 - z_0, z_0$ as can be seen by making the substitutions $u_1 = z_0 - x_0$ and $u_2 = y_0 - z_0$. By obvious extension, any cubic ⟨110⟩ line intersects the five other symmetry-related lines.

(*c*) *Rod axes along ⟨111⟩*. These are perhaps the most interesting, but most difficult to describe and illustrate. There are four invariant structures which again we label with Greek capital letters: (i) Γ: axes u, u, u; $\bar{u}, \frac{1}{2} - u, u$; $\frac{1}{2} + u, \bar{u}, u$; $\frac{1}{2} - u, \frac{1}{2} + u, u$, symmetry $Ia\bar{3}d$. This is probably the densest cubic cylinder packing, with fraction of space filled $\rho = 3^{1/2}\pi/8 = 0.68$. (ii) $^{+}\Sigma$: axes $\frac{1}{3} + u, \frac{2}{3} + u, u$; $\frac{2}{3} - u, \frac{5}{6} - u, u$; $\frac{1}{6} + u, \frac{2}{3} - u, u$; $\frac{5}{6} - u, \frac{5}{6} + u, u$. This second structure is enantiomorphic and $^{-}\Sigma$ has coordinates $\frac{2}{3} + u, \frac{1}{3} + u, u$ *etc*. The symmetry is $I4_132$. The density is 1/9 times that of Γ. (iii) The (non-intersecting) intergrowth of $^{+}\Sigma$ and $^{-}\Sigma$ is labeled Σ^* and has symmetry $Ia\bar{3}d$ and twice the density. (iv) $^{+}\Omega$: axes $\frac{1}{3} + u, \frac{2}{3} + u, u$; $\frac{2}{3} - u, \frac{1}{3} - u, u$; $\frac{2}{3} + u, \frac{2}{3} - u, u$; $\frac{1}{3} - u, \frac{1}{3} + u, u$; symmetry $I432$. The enantiomorph $^{-}\Omega$ has positions $\frac{2}{3} + u, \frac{1}{3} + u, u$ *etc*. In this case, the two enantiomorphs intersect. The density of a cylinder packing with this structure is 4/9 times that of one based on the Γ packing.

O'Keeffe & Andersson (1977) described the first of these structures (Γ) which they named for the garnet structure. It had, in fact, already been mentioned, but not described, by Rosen & Shu (1971). O'Keeffe (1992) added two more, *i.e.* Σ and Σ^*, and discussed the rod symmetries. Ogawa *et al.* (1996) recognized two structures, *i.e.* Γ and Ω, but stated incorrectly that Γ had lower symmetry than Ω. The same two patterns were identified by Parkhouse & Kelly (1998) who did not discuss their symmetries. These last two sets of authors are correct in the sense that Σ and Σ^* can be obtained from Γ by systematic removal of some of the rods, *i.e.* 8/9 and 7/9, respectively.

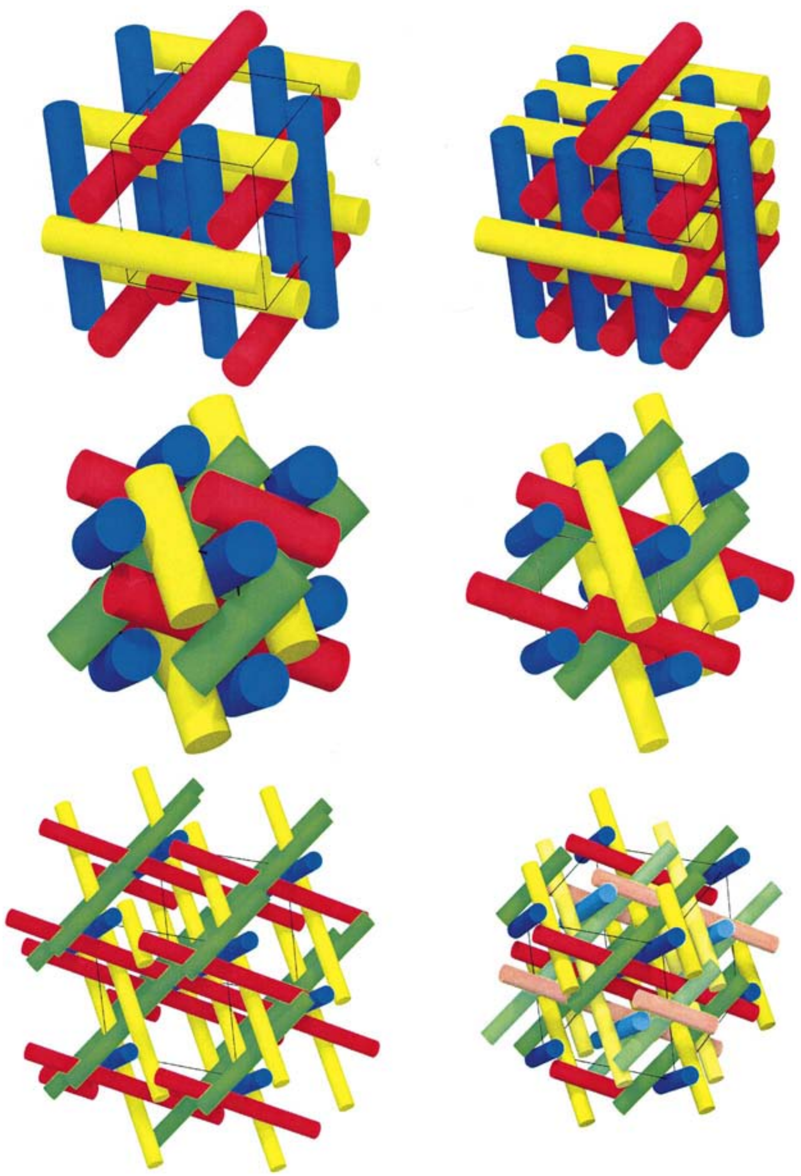

Figure 1
The six invariant cylinder packings. Top row: left $^{+}\Pi$, right Π^{*}. Middle row: left Γ, right $^{+}\Omega$. Bottom row: left $^{+}\Sigma$, right Σ^{*}.

On the other hand, Γ and Ω are fundamentally different in that in Γ the threefold rotation axes (actually $\bar{3}$) do not intersect, but in Ω they do. In Γ the rod axes coincide with the $\bar{3}$ axes (rod symmetry $\mathbf{p}\bar{3}c$) and in $^{+}\Omega$ and $^{-}\Omega$ the rod axes coincide with either the 3_1 or the 3_2 axes (which jointly intersect), with rod symmetry $\mathbf{p}3_1$ or $\mathbf{p}3_2$. Ω describes the axes of a packing of triangular prisms illustrated by Holden (1971) and also described by Parkhouse & Kelly (1998). O'Keeffe (1992) incorrectly associated Σ with that prism packing. Fig. 1 compares the four $\langle 111\rangle$ structures.

O'Keeffe (1992) remarked that the basic cylinder (rod) packings had been identified by looking at crystal structures, so it is interesting that he missed structure Ω. The symmetry $I432$ and its cubic subgroups ($P432$, $P4_232$, $F432$, $F4_132$, $I23$, $P23$, $F23$) are all extremely rare in inorganic crystal chemistry. The Inorganic Crystal Structure Database, which contains about 50000 entries, has 207 entries for these space groups; however, most of them are either clearly wrong (the structures given actually have higher symmetry) or are uncertain (disordered and/or unrefined structures); in particular, the structures of the four entries for $I432$ all actually have symmetry $Im\bar{3}m$. *In toto* there are less than ten authentic structures with these symmetries; none of them appears to be based on the Ω rod packing. The Cambridge Crystal Structure Database, which contains about 200000 mostly molecular crystal structures, has only two examples of structures with symmetry $I432$, and these are both disordered materials; there are correspondingly few entries for the cubic subgroups of $I432$, and most of these are also disordered.

O'Keeffe (1992) described 23 homogeneous cubic cylinder packings, not necessarily in invariant positions; no claim for completeness was made, but we note that there are in fact more than twice this number of homogeneous packings of $\langle 100\rangle$ and $\langle 111\rangle$ cylinders. There is also an innumerable amount of cubic packings of cylinders with axes in sets of 6, 12 and 24 directions. It is planned to describe some of these structures in a separate publication.

This work was supported by the National Science Foundation DMR 98 04817.

References

Audier, M. & Duneau, M. (2000). *Acta Cryst.* A**56**, 49–61.
Duneau, M. & Audier, M. (1999). *Acta Cryst.* A**55**, 746–754.
Fischer, W., Burzlaff, H., Hellner, E. & Donnay, J. H. D. (1973). *Space Groups and Lattice Complexes*, National Bureau of Standards Monograph No. 134. Washington, DC: US Government Printing Office.
Fischer, W. & Koch, E. (1983). *Lattice Complexes*. In *International Tables for Crystallography*, Vol. A, edited by Th. Hahn, pp. 825–854. Dordrecht: Kluwer.
Holden, A. (1971). *Space Shapes and Symmetry*. New York: Columbia University Press.
Ogawa, T., Teshima, Y. & Watanabe, Y. (1995). *Nihon Fukugo Zairo Gakkai Shi* (*J. Jpn. Soc. Compos. Mater.*) **21**, 165–173.
Ogawa, T., Teshima, Y. & Watanabe, Y. (1996). *Katachi U Symmetry*, edited by T. Ogawa, K. Miura, T. Masunari & D. Nagy, pp. 239–246. Tokyo: Springer.
O'Keeffe, M. (1992). *Acta Cryst.* A**48**, 879–884.
O'Keeffe, M. & Andersson, S. (1977). *Acta Cryst.* A**33**, 914–923.
O'Keeffe, M. & Hyde, B. G. (1996). *Crystal Structures I. Patterns and Symmetry*. Washington DC: Mineralogy Society of America.
Parkhouse, J. G. & Kelly, A. (1998). *Proc. R. Soc. London Ser. A*, **454**, 1889–1909.
Rosen, B. W. & Shu, L. S. (1971). *J. Compos. Mater.* **5**, 279–282.