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Homogeneous cubic cylinder packings revisited

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A method of systematically enumerating homogeneous (*i.e.* symmetry-related) packings of equal cylinders is developed. 19 three-way packings with axes parallel to ⟨100⟩ and 40 four-way packings with axes parallel to ⟨111⟩ are described. Cubic 6-, 12- and 24-way packings are possible and examples are given with axes parallel to ⟨210⟩ and ⟨421⟩.

1. Introduction

Homogeneous cylinder packings are periodic structures of equal infinite cylinders in contact with their neighbors, and all related by symmetry. We use the term 'revisited' in our title because an earlier paper with the title *Cubic cylinder packings* (O'Keeffe, 1992) is now known to be incomplete (O'Keeffe *et al.*, 2001). The interest in such structures, which often have remarkable aesthetic appeal (*e.g.* Holden, 1971; Ogawa *et al.*, 1996), arises for a number of reasons. For example, they serve as the basis of periodic structures of fiber-reinforced composite materials (Rosen & Shu, 1971; Ogawa *et al.*, 1995; Parkhouse & Kelly, 1998). They are also of importance in descriptive crystal chemistry (O'Keeffe & Andersson, 1977; O'Keeffe, 1992; Lidin *et al.*, 1995; Sutorik *et al.*, 2000), in the characterization of pore structure in porous materials (Hansen, 1993), and with regard to the arrangement of disclination lattices in the structures of 'blue phases' of cholesteric liquid crystals (Meiboom *et al.*, 1983).

Some of us (see *e.g.* Eddaoudi *et al.*, 2001) are concerned with the design of structures assembled from SBUs (secondary building units). To date, most structures have been assembled from zero-dimensional (finite) SBUs, but attention is now being given to the design and assembly of infinite rod SBUs. It is our thesis (O'Keeffe *et al.*, 2000) that homogeneous structures form the basis for the majority of self-assembled crystalline materials, so it is of considerable interest to know the basic homogeneous structures available. We remark in this connection that the importance of sphere packings in crystal chemistry is commonplace; we expect that cylinder packings will eventually come to play a similar, if subordinate, role. We also expect such structures to be important in the description of ordered self-organizing materials such as polymeric materials (Muthukumar *et al.*, 1997).

In all homogeneous packings described to date, the number of different directions of cylinder axes has been limited to four, but there is considerable interest in packings with more directions (Christensen, 1987; Ogawa *et al.*, 1995) and, for this and for other reasons, quasiperiodic structures based on icosahedral symmetry have been investigated (Ogawa, 1994; Hizume, 1994, 1996; Parkhouse & Kelly, 1998; Duneau & Audier, 1999; Audier & Duneau, 2000). In this paper we describe, we believe for the first time, 6-, 12- and 24-way homogeneous cubic packings.

We start by describing a method for identifying cubic packings of cylinders with axes in an arbitrary set of symmetry-related directions ⟨*uvw*⟩. We give what we believe is a complete list of homogeneous ⟨100⟩ (three-way) and ⟨111⟩ (four-way) packings and their symmetries and coordinates; again a number of these have not been described before. The simplest 6- and 12-way packings are based on ⟨210⟩ and several examples are presented. The simplest 24-way packing appears to be that based on ⟨421⟩ and the three relatively high density structures are also described.

2. Determination of coordinates for cylinder packings

We write a space-group operation in the usual way as a Seitz symbol $(\mathbf{W}|\mathbf{w})$, where $\mathbf{W}$ is the rotation part and $\mathbf{w}$ is the translation part. The coordinates of a point are the column vector $\mathbf{x} = (x/y/z)$, and the direction of a line $[uvw]$ is the direction of the vector $u\mathbf{a} + v\mathbf{b} + w\mathbf{c}$. We write $\mathbf{u}$ for the column vector $(u/v/w)$. Any line is then specified by a point $\mathbf{x}_0 = (x_0/y_0/z_0)$ and $\mathbf{u}_0 = (u_0/v_0/w_0)$. Explicitly, the equations of the line are

$$(x - x_0)/u_0 = (y - y_0)/v_0 = (z - z_0)/w_0. \quad (1)$$

A symmetry operation $(\mathbf{W}_i|\mathbf{w}_i)$ of the space group maps $\mathbf{x}_0$, $\mathbf{u}_0$ to $\mathbf{x}_i$, $\mathbf{u}_i$ where

$$\mathbf{x}_i = \mathbf{W}_i\mathbf{x}_0 + \mathbf{w}_i, \quad \mathbf{u}_i = \mathbf{W}_i\mathbf{u}_0. \quad (2)$$

In the case of cubic structures, we can always choose a reference direction such that $w_0 \neq 0$ so that the line intersects the plane $z = 0$, *i.e.* $z_0 = 0$. Thus any cubic cylinder packing is specified by giving the space group, three integers u_0, v_0 and w_0, specifying the axis direction, and two parameters x_0 and y_0, specifying the intersection with $z = 0$.

The shortest distance between cylinders is readily calculated as da, where a is the cubic unit-cell edge (see Appendix *A*). The density of the packing, defined as the fraction of space occupied by the cylinders, is

$$\rho = n\pi(u_0^2 + v_0^2 + w_0^2)^{1/2} d^2/4, \quad (3)$$

where n is the number of cylinders per unit cell in the set $x_0, y_0, 0$. To find cylinder packings, x_0 and y_0 are varied systematically throughout the unit cell and ρ is calculated. If two cylinders intersect, the density is zero. Likewise, as x_0 and y_0 approach special values where two or more parallel cylinders merge into one, the density approaches zero, until at the special value (cylinders merging) it may again adopt a finite value. The result is that a plot of density in the xy plane has regions of non-zero density separated from each other by lines of zero density, as illustrated in Fig. 1 for ⟨111⟩ cylinders in space group $Ia\bar{3}d$. Inspection shows that invariably each non-zero density region has one clearly defined maximum and decreases monotonically to zero away from the maximum (*i.e.* there were no saddle points; indeed in every case examined the maximum was a cusp with positive curvature at the maximum). Accordingly, we assume that each region surrounded by zero density (these are delta functions for invariant packings) corresponded to just one type of packing and that the stable configuration with maximum kinds of contact was that of the maximum density. With one exception, identified below, the configuration so determined corresponds to a stable packing in which each cylinder is held immobile by its neighbors.

In practice, the calculation proceeds very simply. From one axis at $x_0, y_0, 0$ [uvw], the space-group operations are used to generate the rest of the axes in the unit cell. The distance from one of these to the rest is then calculated. If a zero distance is found then the density is zero; otherwise the shortest distance is found and the density is evaluated according to equation (3). This takes only a small fraction of a second on a desk-top computer. The map in Fig. 1 used a grid of 200 × 200 points and took only a few minutes, and the positions of zeros and maxima are clearly visible. Refinement of the positions requires only the location of a few maxima in one or at most two dimensions. However, it should be noted that the density maps rapidly become more complicated for higher-index directions. Fig. 1 also shows a map for ⟨421⟩ cylinders in $P4_132$; in this case the lines of zero density are barely resolved at 200 × 200 resolution, although the positions of the main maxima are readily apparent. If one wanted to know the total number of distinct packings in such cases, it would appear that the best strategy would be to determine analytically the lines of zero density (it appears that they are always straight lines) and analyze their intersections. However, it is clear that there can be a rather large number of distinct packings and that they are of rather low density, so we have not pursued this aspect of the problem.

There are certain fairly obvious restrictions on the possible symmetry elements compatible with non-zero density packings. In particular, cylinder axes must not be normal to, or intersect, pure rotation axes (as opposed to screw axes) of order greater than two. It follows at once (O'Keeffe *et al.*, 2001) that as all cubic groups have threefold rotation axes there are no non-intersecting cylinder packings for $\langle u_0v_0w_0\rangle$ if any one of $u_0 \pm v_0 \pm w_0 = 0$, such as ⟨110⟩, ⟨321⟩ *etc*. Clearly also, cylinders cannot intersect mirror planes or intersect glide planes with the projection of the cylinder axis on that plane parallel to the glide direction.

Table 1
Symmetries of projection (PG = plane groups) of space groups (SG) on (111).

The seven marked with an asterisk are possible space groups of finite-density ⟨111⟩ cylinder packings. The first set of five rows consists of space groups with non-intersecting threefold axes. The second set of five has intersecting threefold axes.

SG	PG	Others
*$Ia\bar{3}d$	$p6mm$	
*$I4_132$	$p3m1$	$P4_132$, $P4_332$
*$I\bar{4}3d$	$p31m$	
*$Ia\bar{3}$	$p6$	$Pa\bar{3}$
*$I2_13$	$p3$	$P2_13$
$Im\bar{3}m$	$p6mm$	$Pm\bar{3}m$, $Pm\bar{3}n$, $Fm\bar{3}m$, $Fm\bar{3}c$, $Pn\bar{3}m$, $Pn\bar{3}n$, $Fd\bar{3}m$, $Fd\bar{3}c$
*$I432$	$p3m1$	$P432$, $P4_232$, $F432$, $F4_132$
$I\bar{4}3m$	$p31m$	$P\bar{4}3m$, $P\bar{4}3n$, $F\bar{4}3m$, $F\bar{4}3c$
$Im\bar{3}$	$p6$	$Pm\bar{3}$, $Fm\bar{3}$, $Pn\bar{3}$, $Fd\bar{3}$
*$I23$	$p3$	$P23$, $F23$

3. ⟨111⟩ cylinder packings

For non-intersecting rods, the symmetry restrictions mean that there are no non-intersecting ⟨111⟩ cylinder packings for space groups with symbol *.m..*, *.n..*, *.d..*, *...m* or *...c* (note that $P\bar{4}3n$ = $P\bar{4}3c$). For ⟨111⟩ packings, body-centering takes a cylinder into itself, so we can further assert that all such packings are body-centered, and only 7 of the 36 cubic groups are possible symmetries (see Table 1). Except at special positions, the number of cylinders in the unit cell, n in equation (3), is equal to the order of the point group.

The special positions of x_0 and y_0 are the same as the special positions of one of the plane groups (two-dimensional space groups). The plane group in question is just that of the projection of the three-dimensional space group on (111). For example, the projection of $Ia\bar{3}d$ is $p6mm$ and the special and general positions (Wyckoff positions) are: 1(a) (0, 0), 2(b) (1/3, 2/3), 3(c) (0, 1/2), 6(d) (x, 0), 6(e) ($x, \bar{x}$), 12(f) (x, y). The number of cylinders, n, is four times the multiplicity of the Wyckoff position as there are cylinders parallel to [$\bar{1}$11], [1$\bar{1}$1] and [11$\bar{1}$], as well as to [111]. In positions c, a cylinder axis along [111] intersects a threefold axis, so this structure does not correspond to a non-zero density packing. An inspection of the possibilities shows that there are just four distinct (actually six if left- and right-hand enantiomers are distinguished) invariant ⟨111⟩ cylinder packings (O'Keeffe *et al.*, 2001). These are listed in Table 2.

The asymmetric unit for $Ia\bar{3}d$ ⟨111⟩ cylinder packings is that for $p6mm$, *i.e.* the triangle with corners $x_0, y_0 = 0, 0$ and $x_0, y_0 = 1/2, 0$ and $x_0, y_0 = 2/3, 1/3$. This is illustrated in Fig. 2, in which the locations of cylinder packings with a local maximum in density are indicated. Notice that, in $p6mm$, the special position $x, \bar{x}$ belongs to the same set as $2x, x$ (along the line from 0, 0 to 2/3, 1/3 in the figure).

A total of 40 homogeneous ⟨111⟩ cylinder packings were found; these are listed in Tables 2 and 3 and illustrated in projection down [111] in Figs. 3, 4, 5 and 6. There were no new homogeneous packings in $I2_13$ or $I23$ (*i.e.* all packings found in these groups actually had higher symmetry). In 18 of these packings, cylinders are in contact only with cylinders in other orientations (Table 2). In the other 22 packings, two or more parallel cylinders ('bundles') are in contact. Packings of bundles of three or more are given a symbol such as 4–$T3_1$, which means that the individual cylinders of packing number 4 are replaced by the bundle $T3_1$, according to O'Keeffe (1992), whose work may be consulted for illustrations. O'Keeffe (1992) did not recognize the possibility of bundles of two cylinders in ⟨111⟩ packings and these are identified in Fig. 6.

The coordinates of non-bundle packings can all be specified in terms of simple fractions, and they are so listed in Table 2. It is believed that, other than the invariant packings (O'Keeffe *et al.* 2001), these have not been described before, although it is noted that a large model of number 5 has been in Ogawa's laboratory (University of Tsukuba) for a number of years.

All these packings are stable in the sense that a particular cylinder cannot be moved, other than along its axis, without moving an infinite number of others. However, it should be noted that Σ^*, and those with bundles replacing single cylinders of Σ^* (numbers 2, 21, 22 and 34), are composed of two interpenetrating packings based on $^+\Sigma$ and $^-\Sigma$ [the enantio-

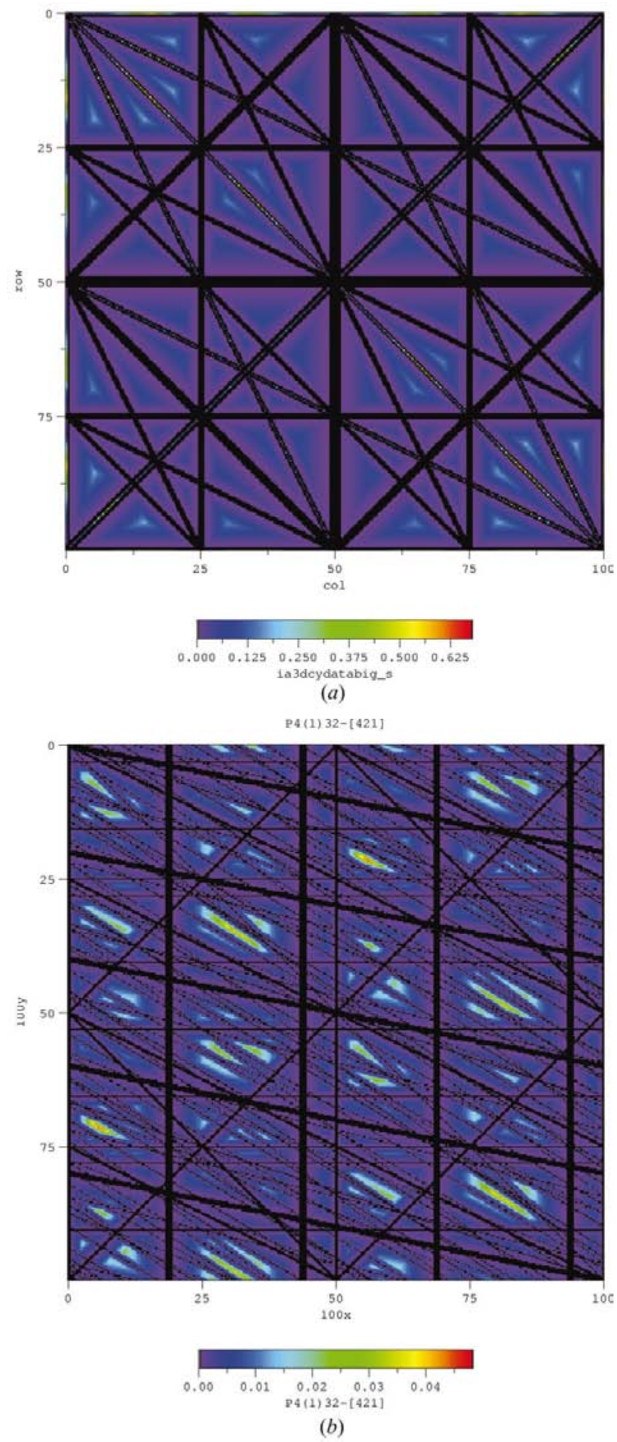

Figure 1
(*a*) The density as a function of x_0 and y_0 for ⟨111⟩ cylinder packings with symmetry $Ia\bar{3}d$. (*b*) The same for ⟨421⟩ cylinder packings with symmetry $P4_132$.

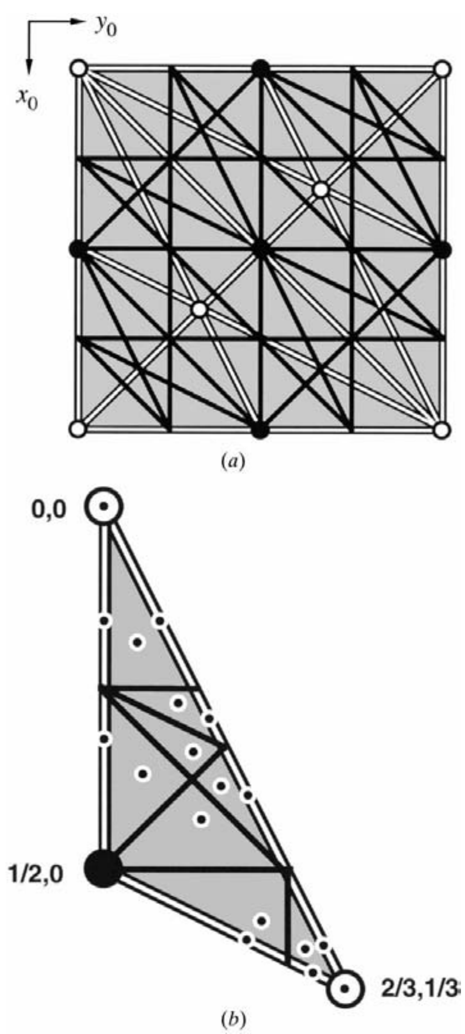

Figure 2
(*a*) The lines of zero density for ⟨111⟩ cylinder packings in $Ia\bar{3}d$ (*cf.* Fig. 1*a*). (*b*) The asymmetric unit of (*a*) with positions of maximum density indicated by filled circles.

Table 2
The invariant (numbers 1 to 4) and non-bundle ⟨111⟩ homogeneous cylinder packings.

The first column contains arbitrary numbers and the symbols are those of O'Keeffe *et al.* (2001). Z is the number of cylinders (of length $3^{1/2}a$) in the unit cell. a is the unit-cell edge for a packing of unit-diameter cylinders and ρ is the fraction of space filled by the cylinders. Structures labelled a and b are enantiomers.

No.	Symbol	SG	x	y	Z	a	ρ
1	Γ	$Ia\bar{3}d$	0	0	4	$2(2^{1/2})$	$3^{1/2}\pi/8$
2	Σ^*	$Ia\bar{3}d$	2/3	1/3	8	$6(2^{1/2})$	$3^{1/2}\pi/36$
3*a*	$^+\Sigma$	$I4_132$	1/3	2/3	4	$6(2^{1/2})$	$3^{1/2}\pi/72$
3*b*	$^-\Sigma$	$I4_132$	2/3	1/3	4	$6(2^{1/2})$	$3^{1/2}\pi/72$
4*a*	$^+\Omega$	$I432$	1/3	2/3	4	$3(2^{1/2})$	$3^{1/2}\pi/18$
4*b*	$^-\Omega$	$I432$	2/3	1/3	4	$3(2^{1/2})$	$3^{1/2}\pi/18$
5		$Ia\bar{3}d$	1/3	0	24	$6(2^{1/2})$	$\pi/4(3^{1/2})$
6		$Ia\bar{3}d$	1/7	6/7	24	$14(2^{1/2})$	$3(3^{1/2})\pi/196$
7		$Ia\bar{3}d$	1/5	4/5	24	$10(2^{1/2})$	$3(3^{1/2})\pi/100$
8		$Ia\bar{3}d$	2/5	3/5	24	$10(2^{1/2})$	$3(3^{1/2})\pi/100$
9*a*		$I4_132$	1/6	5/6	12	$6(2^{1/2})$	$\pi/8(3^{1/2})$
9*b*		$I4_132$	1/6	5/6	12	$6(2^{1/2})$	$\pi/8(3^{1/2})$
10*a*		$I4_132$	2/5	3/5	12	$10(2^{1/2})$	$3(3^{1/2})\pi/200$
10*b*		$I4_132$	3/5	2/5	12	$10(2^{1/2})$	$3(3^{1/2})\pi/200$
11*a*		$I432$	1/5	4/5	12	$5/(2^{1/2})$	$3(3^{1/2})\pi/50$
11*b*		$I432$	4/5	1/5	12	$5/(2^{1/2})$	$3(3^{1/2})\pi/50$
12		$I\bar{4}3d$	1/3	0	12	$6(2^{1/2})$	$\pi/8(3^{1/2})$
13		$Ia\bar{3}d$	1/3	1/9	48	$18(2^{1/2})$	$\pi/18(3^{1/2})$
14		$Ia\bar{3}d$	3/7	1/7	48	$14(2^{1/2})$	$3(3^{1/2})\pi/98$
15		$I\bar{4}3d$	1/3	1/9	24	$18(2^{1/2})$	$\pi/36(3^{1/2})$
16		$I\bar{4}3d$	3/7	1/7	24	$14(2^{1/2})$	$3(3^{1/2})\pi/196$
17		$Ia\bar{3}$	1/3	1/9	24	$18(2^{1/2})$	$\pi/36(3^{1/2})$
18		$Ia\bar{3}$	3/7	1/7	24	$14(2^{1/2})$	$3(3^{1/2})\pi/196$

Table 3
The ⟨111⟩ homogeneous cylinder bundle packings.

The first column contains arbitrary numbers. The symbols are described in the text. Z is the number of cylinders (of length $3^{1/2}a$) in the unit cell. a is the unit-cell edge for a packing of unit-diameter cylinders and ρ is the fraction of space filled by the cylinders.

No.	Symbol	SG	x	y	Z	a	ρ
19	1–$H6_1$	$Ia\bar{3}d$	0.15849	0	24	7.727	0.54675
20	1–$H6_2$	$Ia\bar{3}d$	0.08333	$-x$	24	8.485	0.45345
21	2–$T3_1$	$Ia\bar{3}d$	0.30283	$-x$	24	13.384	0.18225
22	2–$T3_2$	$Ia\bar{3}d$	0.35566	$-x$	24	18.377	0.09668
23	1–$T3_2$	$I4_132$	0.06987	$-x$	12	6.094	0.43951
24	3–$T3_1$	$I4_132$	0.30283	$-x$	12	13.384	0.09113
25	3–$T3_2$	$I4_132$	0.35566	$-x$	12	18.377	0.04834
26	4–$T3_2$	$I432$	0.28868	$-x$	12	9.142	0.19534
27	4–$T3_1$	$I432$	0.39434	$-x$	12	6.692	0.36450
28	1–H3	$I\bar{4}3d$	0.12500	0	12	5.657	0.51013
29	1–H12	$Ia\bar{3}d$	0.19717	0.05283	48	13.384	0.36449
30	2–T6	$Ia\bar{3}d$	0.61383	0.28050	48	23.182	0.12150
31	3–T6	$I4_132$	0.61383	0.28050	24	23.182	0.06075
32	4–T6	$I432$	0.56100	0.22767	24	11.591	0.24300
33		$Ia\bar{3}d$	0.27863	0.11452	48	24.699	0.10704
34		$Ia\bar{3}d$	0.35000	0.05000	48	14.142	0.32648
35		$Ia\bar{3}d$	0.38977	0.16931	48	23.940	0.11393
36		$Ia\bar{3}d$	0.57427	0.21286	48	19.042	0.18009
37		$I4_132$	0.30283	0.10566	24	13.384	0.18225
38		$I4_132$	0.57427	0.21286	24	19.042	0.09005
39		$I432$	0.42573	0.14854	24	9.521	0.36019
40		$I\bar{4}3d$	0.35000	0.05000	24	14.142	0.16324

morphs of the $SrSi_2$ packing (*cf.* O'Keeffe, 1992)] that do not touch each other. Likewise, structure 8 consists of intergrown pairs 10*a* and 10*b* in which cylinders of one set do not touch those of the other. Structures 36 and 38 are derived from 8 and

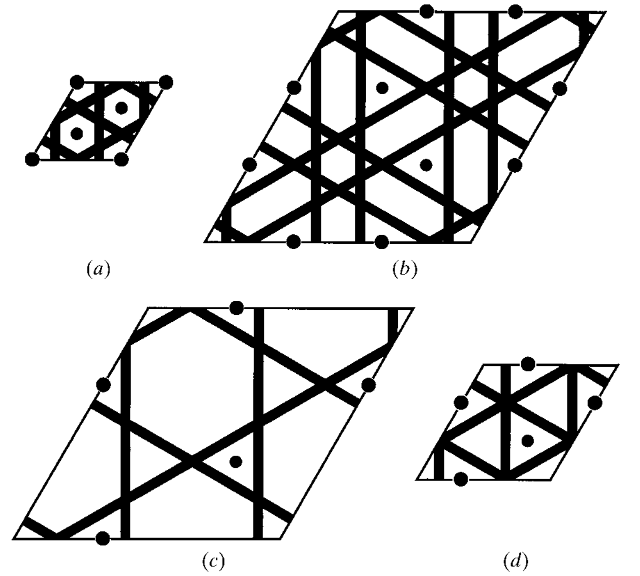

Figure 3
⟨111⟩ cylinder packings viewed down [111]: (*a*)–(*d*) numbers 1–4, respectively. A hexagonal unit cell is outlined.

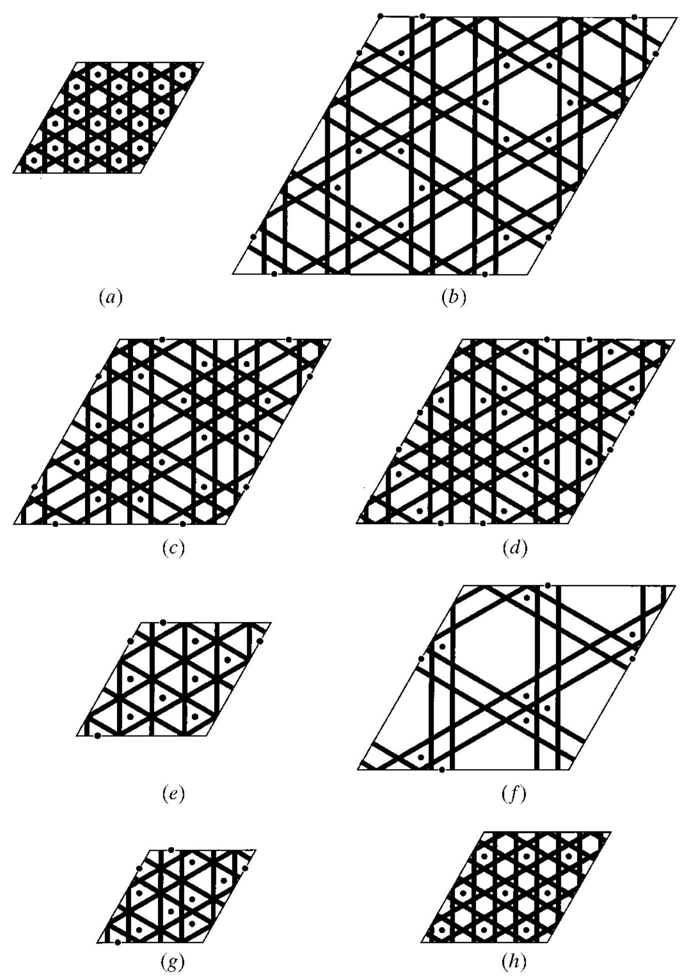

Figure 4
⟨111⟩ cylinder packings viewed down [111]: (*a*)–(*h*) numbers 5–12, respectively. A hexagonal unit cell is outlined.

Table 4
Symmetries of projection (PG = plane groups) of space groups (SG) on (100).

The seven marked with an asterisk are possible space groups of finite density ⟨100⟩ cylinder packings.

SG	PG	Origin	Others
$Im\bar{3}m$	$c4mm$	0, 0	$I\bar{4}3m$, $I432$, $Pn\bar{3}m$, $Pn\bar{3}n$, $Fd\bar{3}c$, $Fd\bar{3}m$
$Pm\bar{3}m$	$p4mm$	0, 0	$P\bar{4}3m$, $P432$, $Fm\bar{3}m$, $Fm\bar{3}c$, $F\bar{4}3c$, $F\bar{4}3m$, $F432$, $Pn\bar{3}m$, $Pn\bar{3}n$
*$Pm\bar{3}n$	$p4mm$	1/2, 0	$P\bar{4}3n$, $P4_232$, $Ia\bar{3}d$, $F4_132$
*$I\bar{4}3d$	$c4gm$	0, 1/4	
*$I4_132$	$c4mm$	1/4, 0	
*$P4_132$	$p4gm$	1/4, 0	
$Im\bar{3}$	$c2mm$	0, 0	$I23$, $Pn\bar{3}$, $Fd\bar{3}$
$Pa\bar{3}$	$p2gm$	0, 0	
*$Pm\bar{3}$	$p2mm$	0, 0	$P23$, $Fm\bar{3}$, $F23$, $Ia\bar{3}$
*$I2_13$	$c2mm$	1/4, 0	
*$P2_13$	$p2gg$	1/4, 0	

10 by replacing each cylinder by a bundle of two cylinders, so 36 is similarly obtained to two interpenetrating enantiomorphs of 38.

4. ⟨100⟩ cylinder packings

The enumeration of these cylinder packings proceeds similarly. Special and general positions are identified from the plane group of the projection of the space group on (100). A small complication, which must be taken into account, is the displacement of the origin of the plane group from that of the space group (using the conventional choice of origin) as indicated in Table 4. For example, for symmetry $Pm\bar{3}m$, the special positions are those of $p4mm$: 1(*a*) (0, 0); 1(*b*) (1/2, 1/2); 2(*c*) (0, 1/2), (1/2, 0). The cylinder axes corresponding to these positions are (*a*) 0, 0, *u*; *u*, 0, 0; 0, *u*, 0; (*b*) 1/2, 1/2, *u*; *u*, 1/2, 1/2; 1/2, *u*, 1/2; (*c*) 0, 1/2, *u*; 1/2, 0, *u*; *u*, 0, 1/2; *u*, 1/2, 0; 1/2, *u*, 0; 0, *u*, 1/2. In each case, the cylinder axes intersect. We note in passing that case (*c*) corresponds to the well known NbO net (O'Keeffe & Hyde, 1996). For space group $Pm\bar{3}n$, the origin is shifted by 0, 1/2 so the cylinder axes become (*a*) 1/2, 0, *u*; *u*, 1/2, 0; 0, *u*, 1/2 and (*b*) 0, 1/2, *u*; *u*, 0, 1/2; 1/2, *u*, 0. Both of these correspond to the invariant packing Π* displaced one from the other by 1/2, 1/2. Positions (*c*) again correspond to the NbO net.

We found the two known invariant packings (O'Keeffe *et al.*, 2001) and three other non-bundle packings (numbers 3, 4 and 5, Table 5), which again we believe have not been published before, although we remark that number 4 ('knight's move') was long known to Ogawa's group. All packings except those with bundles of four or more (identified in Table 6) are illustrated in Figs. 7 and 8.

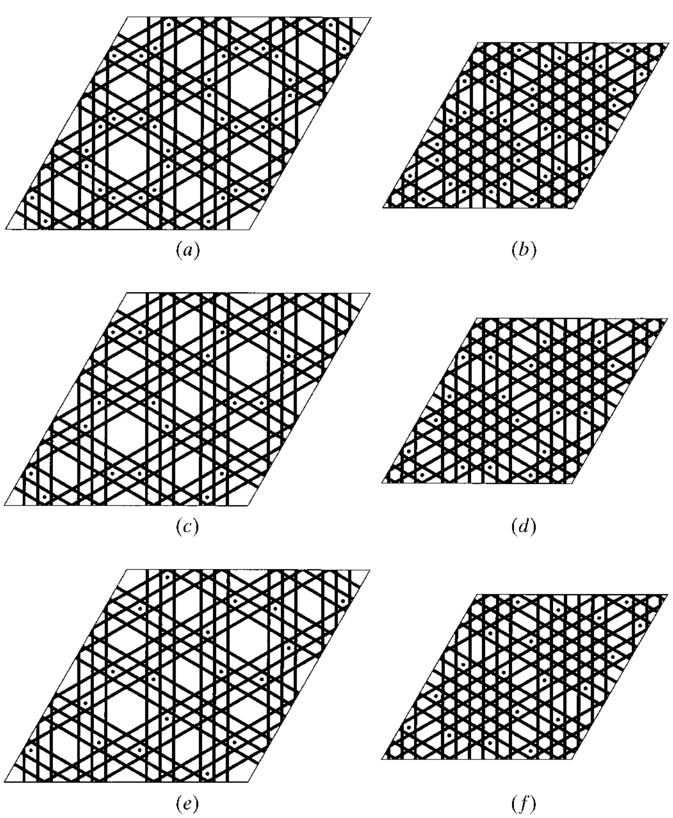

Figure 5
⟨111⟩ cylinder packings viewed down [111]: (*a*)–(*f*) numbers 13–18, respectively. A hexagonal unit cell is outlined.

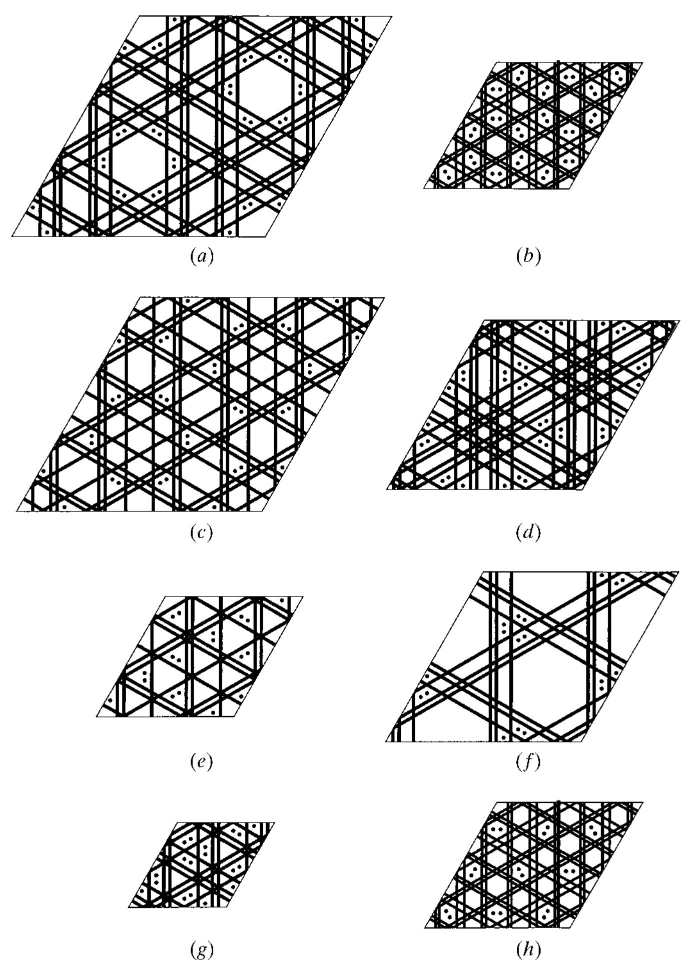

Figure 6
⟨111⟩ cylinder packings, with bundles of two, viewed down [111]: (*a*)–(*h*) numbers 33–40, respectively. A hexagonal unit cell is outlined.

Table 5
The invariant (numbers 1 and 2) and non-bundle ⟨100⟩ cylinder packings.

The first column contains arbitrary numbers and the symbols are those of O'Keeffe *et al.* (2001). Z is the number of cylinders (of length a) in the unit cell. a is the unit-cell edge for a packing of unit-diameter cylinders and ρ is the fraction of space filled by the cylinders.

No.	Symbol	SG	x	y	Z	a	ρ
1	Π^*	$Pm\bar{3}n$	1/2	0	3	2	$3\pi/16$
2a	$^+\Pi$	$I4_132$	1/4	0	6	4	$3\pi/32$
2b	$^-\Pi$	$I4_132$	3/4	0	6	4	$3\pi/32$
3		$I4_132$	2/3	0	12	6	$\pi/12$
4		$I4_132$	1/12	0	24	12	$\pi/24$
5		$I\bar{4}3d$	1/12	0	24	12	$\pi/24$

The ⟨100⟩ packing number 15 is only metastable as any one cylinder can be displaced normal to its axis without displacement of any others.

5. 6-way, 12-way and 24-way cylinder packings

Cubic cylinder packings are also possible for any axes ⟨uvw⟩ for which $u \pm v \pm w \neq 0$. In the general case, there are no finite density packings that correspond to special positions. 6-way packings are possible for ⟨$uv0$⟩ with $u \neq v$ and classes 23 and $m\bar{3}$ (only $Pn\bar{3}$ and $Fd\bar{3}$). We have identified some with relatively high density in the case of ⟨210⟩. As our reference cylinder must intersect the plane $z = 0$, the reference direction is actually [$\bar{2}$01] and the cylinder axes are [201], [20$\bar{1}$], [120], [$\bar{1}$20], [012], [0$\bar{1}$2]. Fig. 9 shows perhaps the simplest and highest density: that with symmetry $P23$ in Table 7.

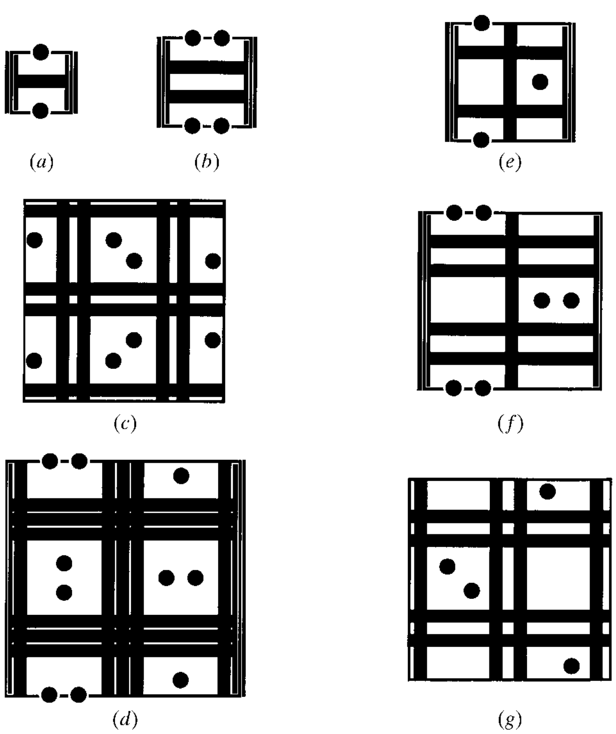

Figure 7
⟨100⟩ cylinder packings viewed down [100]: (*a*) number 1, (*b*) number 18, (*c*) number 11, (*d*) number 15, (*e*) number 2, (*f*) number 19, (*g*) number 17. A unit cell is outlined.

Table 6
The ⟨100⟩ homogeneous cylinder bundle packings.

The first column contains arbitrary numbers. The symbols are described in the text. Z is the number of cylinders (of length a) in the unit cell. a is the unit-cell edge for a packing of unit-diameter cylinders and ρ is the fraction of space filled by the cylinders.

No.	Symbol	SG	x	y	Z	a	ρ
6	1–S4$_2$	$Pm\bar{3}n$	0.35355	0	12	4.840	0.40226
7	1–S4$_1$	$Pm\bar{3}n$	0.125	$1/2 - x$	12	4.000	0.58905
8		$Pm\bar{3}n$	0.18750	0.06250	24	8.000	0.29452
9	1–S8	$Pm\bar{3}n$	0.32322	0.07322	24	6.828	0.40426
10	2–S4$_2$	$I4_132$	0.17678	0	24	9.657	0.20213
11	1–S2	$I4_132$	0.05178	$1/4 - x$	24	6.828	0.40426
12	2–S4$_1$	$I4_132$	0.18750	$1/4 - x$	24	8.000	0.29452
13	4–S2	$I4_132$	0.09375	0.03125	48	16.000	0.14726
14	2–S8	$I4_132$	0.16161	0.03661	48	13.657	0.20213
15		$I\bar{4}3d$	0.18750	0	24	8.000	0.29452
16	5–S2	$I\bar{4}3d$	0.09375	0.03125	48	16.000	0.14726
17	2–S2	$P4_132$	0.18922	$1/4 + x$	12	6.828	0.20213
18		$Pm\bar{3}$	0.33333	0	6	3.000	0.52360
19		$I2_13$	0.16667	0	12	6.000	0.26180

Again with ⟨$uv0$⟩ there are 12-way packings for groups of class 432 for which the fourfold axes are screw axes ($P4_132$, $P4_232$, $P4_332$, $F4_132$ and $I4_132$). A particularly pleasing one

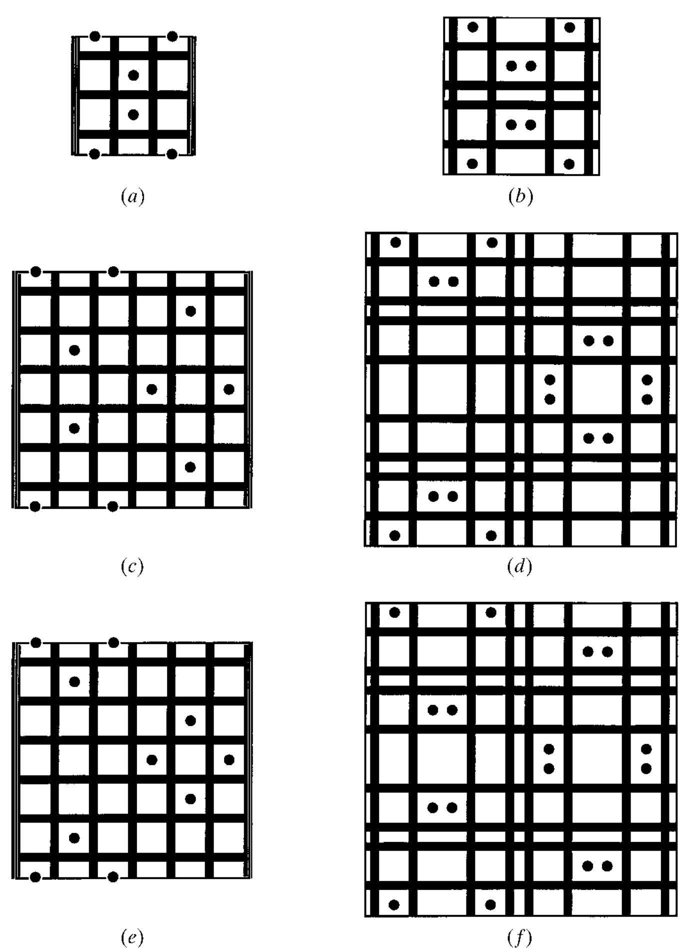

Figure 8
⟨100⟩ cylinder packings viewed down [100]: (*a*) number 3, (*b*) number 8, (*c*) number 4, (*d*) number 13, (*e*) number 5, (*f*) number 16. A unit cell is outlined.

Table 7
Some N-way homogeneous $\langle uvw \rangle$ cylinder packings.

a is the unit-cell edge for a packing of unit-diameter cylinders and ρ is the fraction of space filled by the cylinders.

N	uvw	SG	x	y	a	ρ
6	201	$P23$	0	0.16667	9.165	0.25089
6	201	$P2_13$	0.12500	0.08333	12.220	0.14112
6	201	$Pn\bar{3}$	0.25000	0.18750	14.664	0.19600
12	201	$P4_132$	0.12500	0.44892	16.568	0.15354
12	201	$P4_232$	0	0.19361	10.932	0.35267
24	421	$P432$	0.86581	0.06062	43.490	0.04567
24	421	$P4_132$	0.56085	0.21651	41.809	0.04942
24	421	$P4_232$	0.24028	0.52642	47.129	0.03889

with relatively high density was found with symmetry $P4_232$ (Fig. 10). Although the packing density is quite high, there are large channels through the structure with the arrangement of the Π^* $\langle 100 \rangle$ packing (see the figure) and if these channels are filled with a second set of cylinders of maximum diameter, the combined density of the two packings is 0.692.

For 24-way packings u_0, v_0 and w_0 must all be non-zero and different and the symmetry must be octahedral (in fact only class 432 for finite density). The simplest case is $\langle 421 \rangle$ ($\langle 321 \rangle$ cylinder axes always intersect with cubic symmetry) and the directions are all permutations of [421], [42$\bar{1}$], [4$\bar{2}$1] and [$\bar{4}$21]). These are generally of low density and difficult to illustrate satisfactorily, and we are content to list the three of highest density that we have identified in Table 7.

APPENDIX *A*
The distance between cylinder axes

As explained in the text, we specify a cylinder axis by giving the coordinates x, y, z of a point on the axis and its direction $[uvw]$. For a cubic structure with cell edge a, the shortest distance, d, between two axes x_1, y_1, z_1 $[u_1v_1w_1]$ and x_2, y_2, z_2 $[u_2v_2w_2]$ is computed as follows.

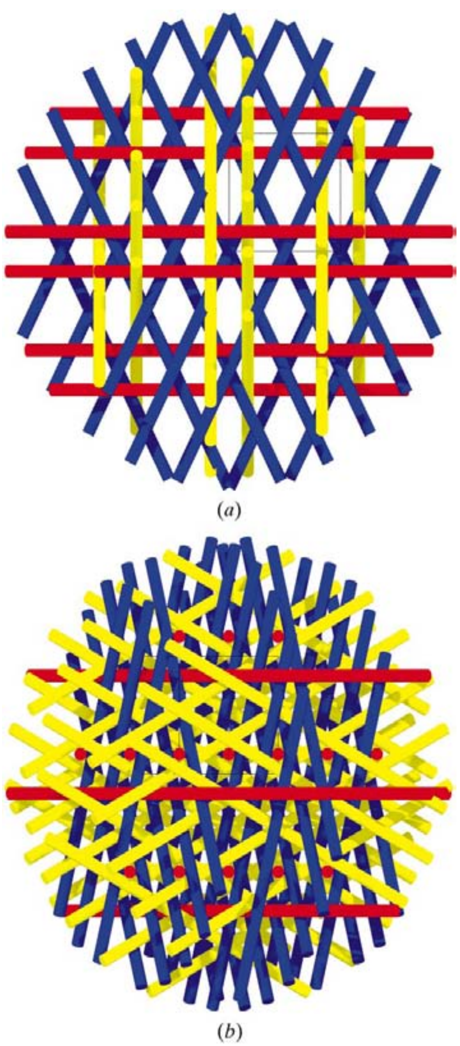

Figure 9
$\langle 201 \rangle$ cylinder packing with symmetry $P23$: (a) viewed down [100], (b) viewed down [120].

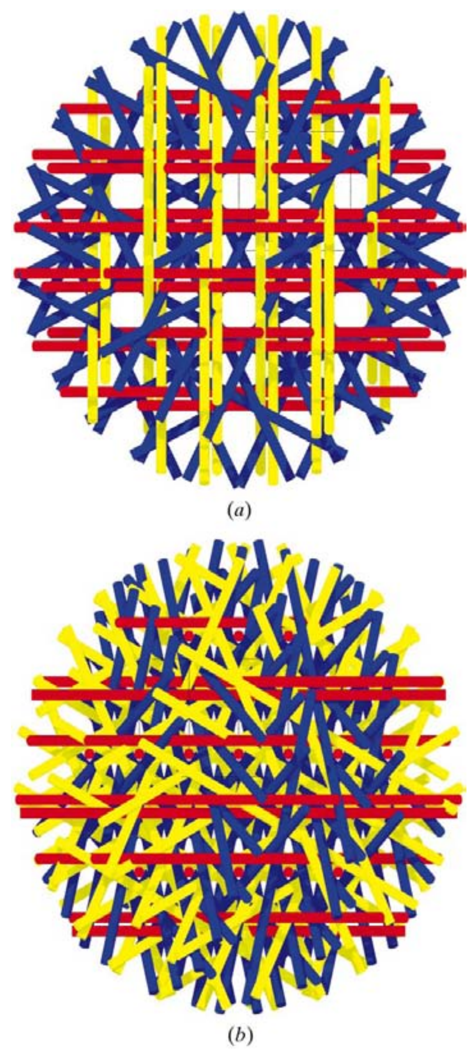

Figure 10
$\langle 201 \rangle$ cylinder packing with symmetry $P4_232$: (a) viewed down [100], (b) viewed down [120].

Let

$$c_1 = u_1(x_1 - x_2) + v_1(y_1 - y_2) + w_1(z_1 - z_2),$$
$$c_2 = u_2(x_1 - x_2) + v_2(y_1 - y_2) + w_2(z_1 - z_2),$$
$$b_1 = u_1^2 + v_1^2 + w_1^2,$$
$$b_2 = u_2^2 + v_2^2 + w_2^2,$$
$$b_{12} = u_1u_2 + v_1v_2 + w_1w_2.$$

For parallel axes,

$$b_1 = b_2 = b_{12}$$

and

$$r_1 = 0,$$
$$r_2 = -c_2/b_2;$$

otherwise

$$r_1 = (c_1b_{12} - c_2b_1)/(b_1b_2 - b_{12}^2),$$
$$r_2 = -(c_2b_{12} - c_1b_2)/(b_1b_2 - b_{12}^2).$$

Then

$$(d/a)^2 = (x_1 + u_1r_1 - x_2 - u_2r_2)^2 + (y_1 + v_1r_1 - y_2 - v_2r_2)^2 + (z_1 + w_1r_1 - z_2 - w_2r_2)^2.$$

The shortest distance from a point x_1, y_1, z_1 to the axis x_2, y_2, z_2 $[u_2v_2w_2]$ is the same as between the parallel axes x_1, y_1, z_1 $[u_2v_2w_2]$ and x_2, y_2, z_2 $[u_2v_2w_2]$.

The coordinates of the point of contact between two equal non-parallel cylinders are

$$x = (x_1 + u_1r_1 + x_2 + u_2r_2)/2,$$
$$y = (y_1 + v_1r_1 + y_2 + v_2r_2)/2,$$
$$z = (z_1 + w_1r_1 + z_2 + w_2r_2)/2.$$

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