9.1. Sphere packings and packings of ellipsoids

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9.1.1. Sphere packings and packings of circles

9.1.1.1. *Definitions*

For the characterization of many crystal structures, geometrical aspects have proved to be a useful tool. Among these, sphere-packing considerations stand out in particular.

A *sphere packing* in the most general sense is an infinite, three-periodic set of non-intersecting spheres (*i.e.* a set of non-intersecting spheres with space-group symmetry) with the property that any pair of spheres is connected by a chain of spheres with mutual contact. If all spheres are symmetry-equivalent, the sphere packing is called *homogeneous*, otherwise it is called *heterogeneous*.

A homogeneous sphere packing may be represented uniquely by the set of symmetry-equivalent points that are the centres of the spheres [point configuration, *cf. IT*A (1983, Chapter 14.1)]. This point configuration is distinguished by equal shortest distances giving rise to a connected graph. As all spheres of a homogeneous sphere packing must be equal in size, their common radius can be calculated as half this shortest distance.

A heterogeneous sphere packing consists of at least two symmetry-distinct subsets of spheres, the centres of which form a respective number of point configurations. The radii of symmetrically distinct spheres can be either equal or different. In the first case, the heterogeneous sphere packing may be represented by its set of sphere centres, quite similar to a homogeneous one. In the case of different sphere radii, however, the knowledge of at least some of the radii is additionally necessary.

As there exists an infinite number of both homogeneous and heterogeneous sphere packings, it is convenient to classify the sphere packings into types: two sphere packings belong to the same *type* if there exists a biunique mapping that brings the spheres of one packing onto the spheres of the other packing and that preserves all contact relations between spheres.

The number of types of homogeneous sphere packings is finite whereas the number of types of heterogeneous sphere packings is infinite.

All definitions and properties mentioned so far may be transferred from sets of spheres in three-dimensional space to sets of circles in two-dimensional space, giving rise to *heterogeneous* and *homogeneous packings of circles*.

A characteristic property of types of homogeneous sphere (circle) packings is the number k of contacts per sphere (circle): $3 \le k \le 12$ for sphere packings and $3 \le k \le 6$ for packings of circles.

A sphere (circle) packing is called *stable* [close, *cf. IT* II (1972, Chapter 7.1)] if no sphere (circle) can be moved without moving neighbouring spheres (circles) at the same time. As a consequence, a stable sphere (circle) packing has at least four (three) contacts per sphere (circle), and not all these contacts must fall in one hemisphere (semicircle).

The *density* of a homogeneous sphere (circle) packing is defined as the fraction of volume (area) occupied by spheres (circles). It may be calculated as

$$\rho = \tfrac{4}{3}\pi \frac{nr^3}{V}$$

for sphere packings, and as

$$\rho = \pi \frac{nr^2}{A}$$

for packings of circles. Here, r is the radius of the spheres (circles), n the number of spheres (circles) per unit cell, V the unit-cell volume, and A the unit-cell area.

Geometric properties of different sphere (circle) packings of the same type may be different. Such properties are, *e.g.*, the density and the property of being a stable packing.

9.1.1.2. *Homogeneous packings of circles*

The homogeneous packings of circles in the plane may be classified into 11 types (*cf.* Niggli, 1927, 1928; Haag, 1929, 1937; Sinogowitz, 1939; Fischer, 1968; Koch & Fischer, 1978). These correspond to the 11 types of planar nets with equivalent vertices derived by Shubnikov (1916). If, in addition, symmetry is used for classification, the number of distinct cases becomes larger (31 cases according to Sinogowitz, 1939).

Table 9.1.1.1 gives a summary of the 11 types. In column 1, the type of circle packing is designated by a modified Schläfli symbol that characterizes the polygons meeting at one vertex of a corresponding Shubnikov net. The contact number k is given in column 2. The next column displays the highest possible symmetry for each type of circle packing. The corresponding parameter values are listed in column 4. The appropriate shortest distances d between circle centres and densities ρ are given in columns 5 and 6, respectively.

With three exceptions (3^6, $3^4 6$, 46.12), all types include circle packings that are not similar in the mathematical sense and that differ, therefore, in their geometrical properties. The highest possible symmetry for a type of homogeneous circle packing corresponds necessarily to the lowest possible density ρ of that type. Therefore, homogeneous circle packings of type 3.12^2 with symmetry $p6mm$ are the least dense. The highest possible density is achieved by the circle packings with contact number 6 referring to triangular nets with hexagonal symmetry.

All circle packings described in Table 9.1.1.1 are stable in the sense defined above. Only circle packings of types 3.12^2 and 48^2 may be unstable.

9.1.1.3. *Homogeneous sphere packings*

The number of homogeneous sphere-packing types is not known so far. Sinogowitz (1943) systematically derived sphere packings with non-cubic symmetry from planar sets of spheres, but he did not compare sphere packings with different symmetry and classify them into types. Fischer calculated the parameter conditions for all cubic (Fischer, 1973, 1974) and all tetragonal (Fischer, 1991a,b, 1993) sphere packings. 199 types of homogeneous sphere packings with cubic symmetry and 394 types with tetragonal symmetry exist in all. 12 of these types are common to both systems. In a similar way, Zobetz (1983) calculated the sphere-packing conditions for Wyckoff position $R\bar{3}m$ $6(c)$. Using a different approach, Koch & Fischer (1995) derived all types of homogeneous sphere packings with contact number $k = 3$. Because of the unique correspondence of each homogeneous sphere packing to a graph, studies on three-dimensional nets also give contributions to the knowledge on sphere-packing types. In particular, papers by Wells (1977, 1979, 1983), O'Keeffe (1991, 1992), O'Keeffe & Brese (1992) and Treacy, Randall, Rao, Perry & Chadi (1997) contain some information on sphere packings with $k = 3$ and $k = 4$.

Table 9.1.1.1. *Types of circle packings in the plane*

Type	k	Symmetry			Parameters	Distance d	Density
3^6	6	$p6mm$	$1(a)$	$0, 0$		a	0.9069
3^2434	5	$p4gm$	$4(c)$	$x, x+\frac{1}{2}$	$x=\frac{1}{4}\sqrt{3}-\frac{1}{4}$	$\frac{1}{2}(\sqrt{6}-\sqrt{2})a$	0.8418
3^34^2	5	$c2mm$	$4(d)$	$x, 0$	$x=1-\frac{1}{2}\sqrt{3}; b/a=2-\sqrt{3}$	b	0.8418
3^46	5	$p6$	$6(d)$	x, y	$x=\frac{3}{7}; y=\frac{1}{7}$	$\frac{1}{7}\sqrt{7}a$	0.7773
4^4	4	$p4mm$	$1(a)$	$0, 0$		a	0.7854
3464	4	$p6mm$	$6(e)$	$x, \bar{x}$	$x=\frac{1}{2}-\frac{1}{6}\sqrt{3}$	$\frac{1}{2}(\sqrt{3}-1)a$	0.7290
3636	4	$p6mm$	$3(c)$	$\frac{1}{2}, 0$		$\frac{1}{2}a$	0.6802
6^3	3	$p6mm$	$2(b)$	$\frac{1}{3}, \frac{2}{3}$		$\frac{1}{3}\sqrt{3}a$	0.6046
48^2	3	$p4mm$	$4(d)$	$x, 0$	$x=1-\frac{1}{2}\sqrt{2}$	$(\sqrt{2}-1)a$	0.5390
46.12	3	$p6mm$	$12(f)$	x, y	$x=\frac{1}{6}\sqrt{3}+\frac{1}{6}; y=\frac{1}{6}\sqrt{3}-\frac{1}{6}$	$(\frac{1}{2}-\frac{1}{6}\sqrt{3})a$	0.4860
3.12^2	3	$p6mm$	$6(c)$	$x, \bar{x}$	$x=1-\frac{1}{3}\sqrt{3}$	$(2-\sqrt{3})a$	0.3907

Table 9.1.1.2 shows examples for sphere packings with high contact numbers and high densities in the upper part and with small contact numbers and low densities in the lower part. Column 1 gives reference numbers to designate the types in the following. Column 2 displays the contact numbers k. The highest possible symmetry for each type is described in column 3. Coordinates and metrical parameters referring to the most regular sphere packings of each type are listed in column 4; the respective shortest distances d between sphere centres are given in column 5. For a sphere packing that can be subdivided into plane nets of spheres with mutual contact, the direction and the type of these nets are shown in column 6. Column 7 contains stacking information: the contact numbers to the nets above and below, and the number of layers per translation period in the direction perpendicular to the layers. The last column displays the density with respect to the parameters of column 4. For all cases, this value gives the minimal density for that type of sphere packing.

The densest homogeneous sphere packings known so far may be derived from the densest packings of circles (3^6 in Table 9.1.1.1). Such sphere packings can always be subdivided into parallel plane layers of spheres with six contacts per sphere within each layer and with three contacts to each of the neighbouring layers above and below (*cf.* Fig. 9.1.1.1). Consequently, the contact number k becomes 12. As there exist two stacking possibilities for each layer with respect to the previous layer, infinitely many stacking sequences can be derived in principle, but only two refer to homogeneous sphere packings. If for each layer the two neighbouring layers are stacked directly upon each other, a sphere packing of a two-layer type with hexagonal symmetry (type 1) results. It is called *hexagonal closest packing* (abbreviated h.c.p.). If for all layers the neighbouring layers are never stacked directly upon each other, a sphere packing of a three-layer type with cubic symmetry (type 2) is formed. It is designated *cubic closest packing* (c.c.p.). In spite of these terms, for a long time it was only known that the cubic closest packings are the densest ones that correspond to lattices (Minkowski, 1904). Only recently, Hsiang (1993) published a proof that there does not exist any packing of spheres of equal size with a higher density, but the completeness of this proof is still doubted (*cf. e.g.* Hales, 1994).

Independently of the stacking sequences, closest packings of spheres contain ideal octahedral and ideal tetrahedral voids. The number of octahedra per unit cell equals the respective number of spheres, whereas the number of tetrahedral voids is twice as large. The distances between the centres and the vertices of these voids are $\sqrt{2}d/2$ and $\sqrt{6}d/4$, respectively. Within a cubic closest packing, faces are shared only between octahedral and tetrahedral voids. Each edge is common to two octahedra and two tetrahedra. In contrast, piles of face-sharing octahedra are formed within a hexagonal closest packing, whereas the tetrahedra are arranged as pairs with one face in common. The other faces are shared between octahedra and tetrahedra. Again, each edge belongs to two octahedra and two tetrahedra.

Densest layers of spheres may also be stacked such that each sphere is in contact with two spheres of the previous layers (*cf.* Fig. 9.1.1.2). Such a stacking results in contact number 10. Again, infinitely many periodic stacking sequences are possible, but only four give rise to homogeneous sphere packings [types 9, 10, 11: *cf.* Hellner (1986); type 12: *cf.* O'Keeffe (1988)]. In the most symmetrical forms of these four cases, each sphere is located exactly above or below the middle of two neighbouring spheres of the adjacent layers. This kind of stacking gives rise to distorted tetrahedral voids only. The number of tetrahedra per unit cell is six times the number of spheres. Two kinds of differently distorted tetrahedra exist in the ratio 1:2. The two-layer type 9 corresponds to a tetragonal body-centred lattice with specialized axial ratio.

Furthermore, densest layers of spheres may be stacked in a mixed sequence with three contacts per sphere to one neighbouring layer and two contacts to the other layer. This kind of stacking results in five types of homogeneous sphere packings (3 to 7) with contact number 11.
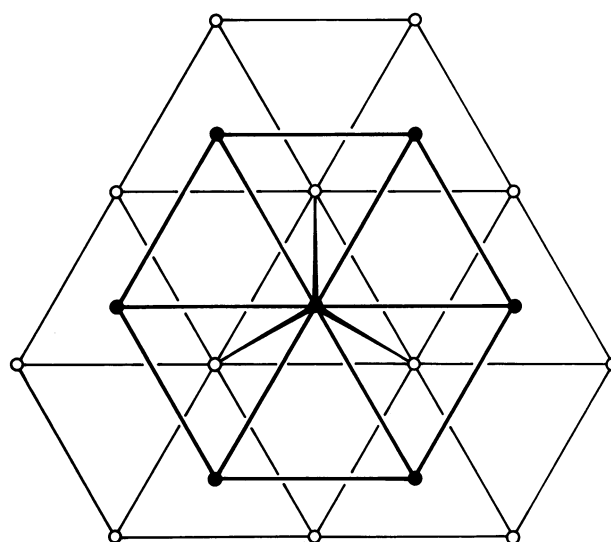

Fig. 9.1.1.1. Two triangular nets representing two densest packed layers of spheres. The layers are stacked in such a way that each sphere is in contact with three spheres of the other layer.

Table 9.1.1.2. *Examples for sphere packings with high contact numbers and high densities and with low contact numbers and low densities*

Type	k	Symmetry			Parameters	Distance d	Net	Stacking	Density
1	12	$P6_3/mmc$	$2(c)$	$\frac{1}{3},\frac{2}{3},\frac{1}{4}$	$c/a=\frac{2}{3}\sqrt{6}$	a	$(001)\ 3^6$	3, 3 2	0.7405
2	12	$Fm\bar{3}m$	$4(a)$	$0,0,0$	–	$\frac{1}{2}\sqrt{2}a$	$\{111\}\ 3^6$	3, 3 3	
							$\{001\}\ 4^4$	4, 4 2	
3	11	$Cmca$	$8(f)$	$0,y,z$	$y=\frac{1}{6},z=\frac{3}{2}\sqrt{2}-2$	a	$(001)\ 3^6$	3, 2 4	0.7187
					$b/a=\sqrt{3},c/a=\frac{2}{3}\sqrt{6}+\sqrt{3}$				
4	11	$P3_121$	$6(c)$	x,y,z	$x=\frac{1}{2},y=\frac{5}{6},z=\sqrt{2}-\frac{4}{3}$	a	$(001)\ 3^6$	3, 2 6	
					$c/a=\sqrt{6}+\frac{3}{2}\sqrt{3}$				
5	11	$Fdd2$	$16(b)$	x,y,z	$x=\frac{1}{6},y=\frac{3}{4}\sqrt{2}-1,z=0$	c	$(010)\ 3^6$	3, 2 8	
					$b/a=\frac{4}{3}\sqrt{2}+2,c/a=\frac{1}{3}\sqrt{3}$				
6	11	$P6_522$	$12(c)$	x,y,z	$x=\frac{1}{6},y=\frac{1}{3},z=\frac{1}{2}\sqrt{2}-\frac{2}{3}$	a	$(001)\ 3^6$	3, 2 12	
					$c/a=2\sqrt{6}+3\sqrt{3}$				
7	11	$C2/m$	$4(i)$	$x,0,z$	$x=\frac{1}{2}\sqrt{2}-\frac{1}{2},z=3\sqrt{2}-4$	b	$(001)\ 3^6$	3, 2 12	
					$b/a=\frac{1}{3}\sqrt{3},c/a=\frac{1}{6}\sqrt{6}+\frac{1}{3}\sqrt{3}$				
					$\cos\beta=\frac{1}{6}\sqrt{6}-\frac{1}{3}\sqrt{3}$				
8	11	$P4_2/mnm$	$4(f)$	$x,x,0$	$x=\frac{1}{2}\sqrt{2}-\frac{1}{2},c/a=2-\sqrt{2}$	c	–	–	0.7187
9	10	$I4/mmm$	$2(a)$	$0,0,0$	$c/a=\frac{1}{3}\sqrt{6}$	c	$\{110\}\ 3^6$	2, 2 2	0.6981
10	10	$P6_222$	$3(c)$	$\frac{1}{2},0,0$	$c/a=\frac{3}{2}\sqrt{3}$	a	$(001)\ 3^6$	2, 2 3	
11	10	$Fddd$	$8(a)$	$0,0,0$	$b/a=\sqrt{3},c/a=2\sqrt{3}$	a	$(001)\ 3^6$	2, 2 4	
12	10	$Fddd$	$16(g)$	$\frac{1}{8},\frac{1}{8},z$	$z=\frac{5}{16},b/a=\sqrt{3},c/a=4\sqrt{3}$	a	$(001)\ 3^6$	2, 2 8	
13	10	$Cmcm$	$4(c)$	$0,y,\frac{1}{4}$	$y=\frac{3}{10},b/a=\frac{1}{3}\sqrt{15},c/a=\frac{2}{5}\sqrt{10}$	$\frac{1}{3}\sqrt{6}a$	$(001)\ 4^4$	3, 3 2	0.6981
14	10	$Pnma$	$4(c)$	$x.\frac{1}{4},z$	$x=\frac{7}{20},z-\frac{7}{8},b/a=\frac{4}{5},c/a=\frac{2}{15}\sqrt{15}$	c	$(010)\ 4^4$	3, 3 2	
15	10	$P6_3/mmc$	$4(f)$	$\frac{1}{3},\frac{2}{3},z$	$z=\frac{3}{4}-\frac{1}{4}\sqrt{6},c/a=\frac{2}{3}\sqrt{6}+2$	a	$(001)\ 3^6$	3, 1 4	0.6657
16	10	$R\bar{3}m$	$6(c)$	$0,0,z$	$z=\frac{1}{2}-\frac{1}{6}\sqrt{6},c/a=\sqrt{6}+3$	a	$(001)\ 3^6$	3, 1 6	
17	10	$Cmcm$	$4(c)$	$0,y,\frac{1}{4}$	$y=\frac{3}{4}-\frac{1}{4}\sqrt{6},$	a	$(010)\ 4^4$	4, 2 4	0.6657
					$c/a=1,b/a=\sqrt{3}+\sqrt{2}$				
18	10	$I4_1/amd$	$8(e)$	$0,0,z$	$z=\frac{1}{2}-\frac{1}{8}\sqrt{6},c/a=2\sqrt{3}+2\sqrt{2}$	a	$(001)\ 4^4$	4, 2 8	
19	10	$I4/m$	$8(h)$	$x,y,0$	$x=\frac{6}{17}-\frac{1}{17}\sqrt{2},y=\frac{7}{17}-\frac{4}{17}\sqrt{2}$	c	–	–	0.6619
					$c/a=(\frac{14}{17}-\frac{8}{17}\sqrt{2})^{1/2}$				
20	10	$R\bar{3}$	$18(f)$	x,y,z	$x=\frac{3}{7},y=\frac{1}{7},z=0,c/a=\frac{1}{7}\sqrt{42}$	$\frac{1}{7}\sqrt{7}a$	(001) 3^46	3, 2 3	0.6347
21	4	$Fd\bar{3}m$	$32(e)$	x,x,x	$x=\frac{3}{8}-\frac{1}{8}\sqrt{6}$	$(\frac{3}{4}\sqrt{2}-\frac{1}{2}\sqrt{3})a$	–	–	0.1235
22	4	$Im\bar{3}m$	$48(j)$	$0,y,z$	$y=\frac{4}{7}-\frac{3}{28}\sqrt{2},z=\frac{5}{14}-\frac{1}{28}\sqrt{2}$	$(\frac{3}{14}\sqrt{2}-\frac{1}{7})a$	–	–	0.1033
23	4	$I4_132$	$48(i)$	x,y,z	$x=y=\frac{1}{8}\sqrt{2},z=0$	$(\frac{1}{2}-\frac{1}{4}\sqrt{2})a$	–	–	0.0789
24	3	$I4_132$	$24(h)$	$\frac{1}{8},y,\frac{1}{4}-y$	$y=\frac{1}{4}\sqrt{3}-\frac{3}{8}$	$(\frac{1}{2}\sqrt{6}-\frac{3}{4}\sqrt{2})a$	–	–	0.0555

Two other types of homogeneous sphere packings (15 and 16) with contact number $k = 10$ also refer to densest layers of spheres. In these cases, each sphere has three contacts to one neighbouring layer and one contact to the other layer that is stacked directly above or below the original layer.

Cubic closest packings may also be regarded as built up from square layers 4^4 stacked in such a way that each sphere has four neighbouring spheres in the same layer and four neighbours each from the layers above and below (cf. Fig. 9.1.1.3). If square layers are stacked such that each sphere has contact to four spheres of one neighbouring layer and to two spheres of the other layer (cf. Fig. 9.1.1.4), sphere packings with contact number 10 result. In total, two types of homogeneous packings (17 and 18) with this kind of stacking exist. Sphere packings of type 9 may also be decomposed into 4^4 layers parallel to (101) or (011) in a five-layer sequence. These nets are made up from parallel rhombi and stacked such that each sphere has contact with three other spheres from the layer above and from the layer below. If such layers are stacked in a two-layer sequence, sphere packings of type 13

with symmetry *Cmcm* result (O'Keeffe, 1998). Sphere packings of type 14 are also build up from 4^4 layers, but here the rhombi occur in two different orientations (O'Keeffe, 1998). Sphere packings with high contact numbers may also be derived by stacking of other layers. Type 20, for example, refers to $3^4 6$ layers where each sphere is in contact with three spheres of one neighbouring net and two spheres of the other one (Sowa & Koch, 1999). Such a sphere packing may alternatively be derived from the cubic closest packing by omitting systematically $1/7$ of the spheres in each of the 3^6 nets.

Sphere packings of types 8 and 19 (cf. Figs. 9.1.1.5 and 9.1.1.6) cannot be built up from plane layers of spheres in contact although their contact numbers are also high.

Table 9.1.1.2 contains complete information on homogeneous sphere packings with $k = 10$, 11, and 12 and with cubic or tetragonal symmetry.

The least dense (most open) homogeneous sphere packings known so far have already been described by Heesch & Laves (1933). Sphere packings of that type (24) cannot be stable because their contact number is 3 (cf. Fig. 9.1.1.7). As discussed
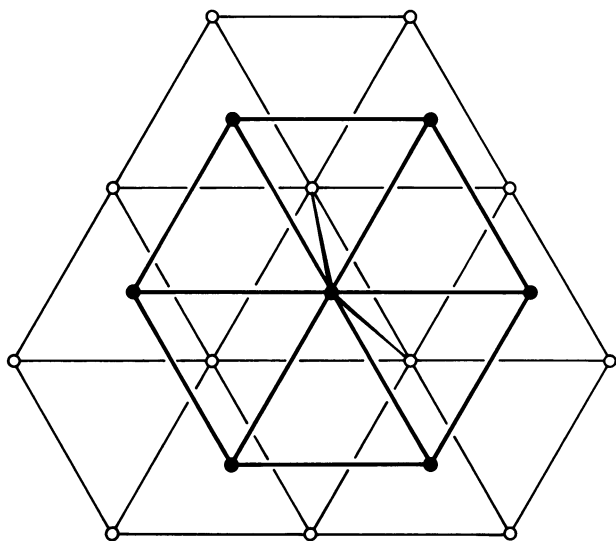

Fig. 9.1.1.2. Two triangular nets representing two densest packed layers of spheres. The layers are stacked in such a way that each sphere is in contact with two spheres of the other layer.
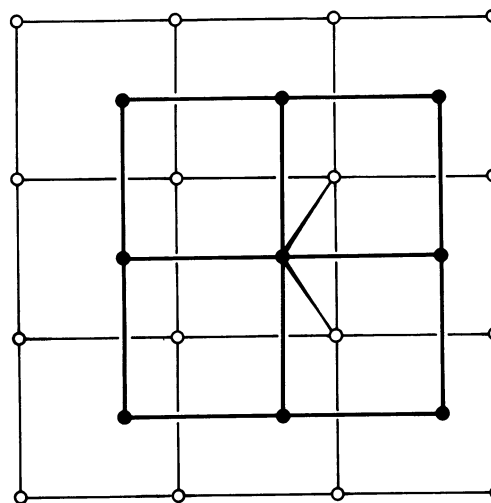

Fig. 9.1.1.4. Two square nets representing two layers of spheres stacked in such a way that each sphere is in contact with two spheres of the other layer.
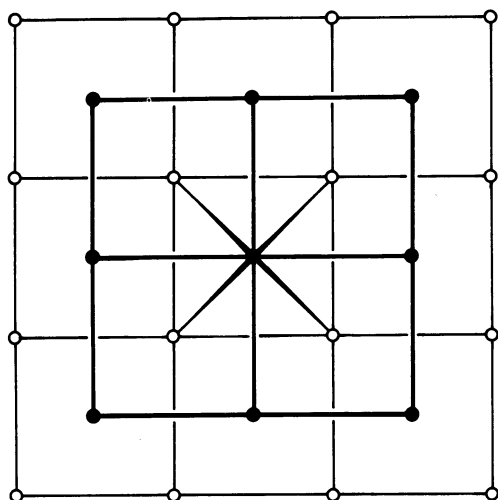

Fig. 9.1.1.3. Two square nets representing two layers of spheres stacked in such a way that each sphere is in contact with four spheres of the other layer.
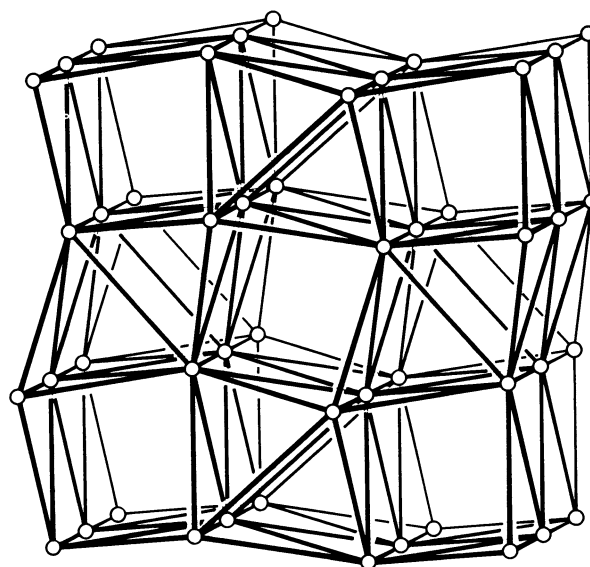

Fig. 9.1.1.5. Sphere packing of type 8 (Table 9.1.1.2) represented by a graph: $k = 11$, $P4_2/mnm$, $4(f)$, $xx0$.

by Fischer (1976), it is very probable that no homogeneous sphere packings with lower density exist; those discussed by Melmore (1942*a*,*b*) with $\rho = 0.042$ and $\rho = 0.045$ are heterogeneous ones. Recently, Koch & Fischer (1995) proved that the Heesch–Laves packing is the least dense homogeneous sphere packing with three contacts per sphere.

The least dense sphere packings with contact number 4 derived so far are described as type 23. All sphere packings of this type are similar in the geometrical sense and are not stable. In contrast, the sphere packings of type 22 are stable. Sphere packings of type 21 (Heesch & Laves, 1933), which have been supposed to be the most open stable ones (*cf.* Hilbert & Cohn-Vossen, 1932, 1952), have a slightly higher density.

On the basis of the material known at that time, Slack (1983) tried to develop empirical formulae for the minimal and the maximal density of circle packings and sphere packings depending on the contact number. A paper by O'Keeffe (1991) on four-connnected nets pays special attention to the densest and the least dense sphere packings with four contacts per sphere.

9.1.1.4. *Applications*

Sphere packings have been used for the description of inorganic crystal structures in different ways and by several authors (*e.g.* Brunner, 1971; Figueiredo & Lima-de-Faria, 1978; Frank & Kasper, 1958; Hellner, 1965; Hellner, Koch & Reinhardt, 1981; Koch, 1984, 1985; Laves, 1930, 1932; Lima-de-Faria, 1965; Lima-de-Faria & Figueiredo, 1969*a*,*b*; Loeb, 1958; Morris & Loeb, 1960; Niggli, 1927; Smirnova, 1956*a*,*b*, 1958*a*,*b*, 1959*a*,*b*,*c*, 1964; Sowa, 1988, 1997).

In the simplest case, the structure of an element may be described as a sphere packing if all atoms are interrelated by equal or almost equal shortest distances. This does not imply that the atoms really have to be considered as hard spheres of that size. Often such sphere packings are homogeneous ones with a high contact number k (*e.g.* Cu, Mg with $k = 12$; Pa with $k = 10$; W with $k = 8$). Low values of k (*e.g.* diamond with $k = 4$, white tin with $k = 6$) and heterogeneous sphere packings (La with $k = 12$) have also been observed for structures of elements.
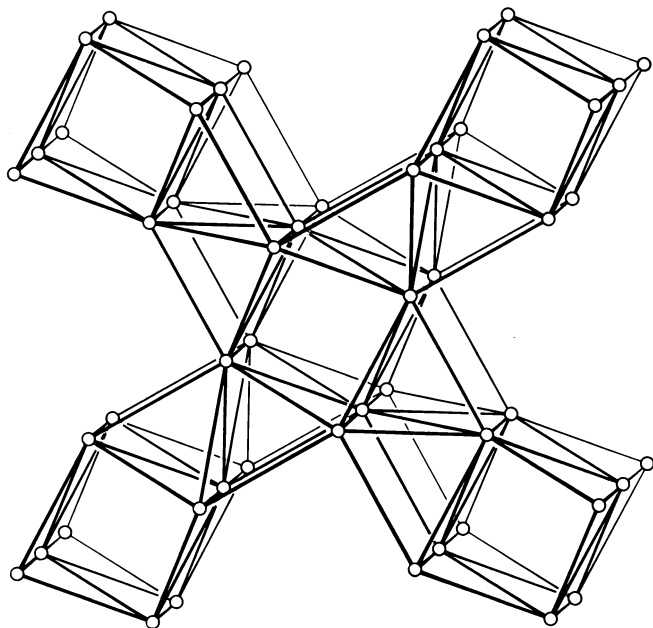
Crystal structures consisting of different atoms may be related to sphere packings in different ways:

(1) The structure as a whole may be considered as a heterogeneous sphere packing. In that case, contacts at least between different spheres are present (*e.g.* CsCl, NaCl, CaF_2). In addition, contacts between equal atoms may exist (I—I contacts in CsI) or may even be necessary (CdI_2). In general, a type of heterogeneous sphere packing is compatible with a certain range of radius ratios (*cf.* alkali halides). In special cases, a heterogeneous sphere packing may be derived from a homogeneous one by subgroup degradation (*e.g.* NaCl, CsCl, PtCu).

(2) Part of the crystal structure, *e.g.* the anions or the more frequent kind of atoms, may be considered as a sphere packing whereas the other atoms are located within the voids of that sphere packing. For this approach, the atoms corresponding to the sphere packing need not necessarily be in contact (*cf. e.g.* the Cl—Cl distances in NaCl and LiCl). Voids within sphere packings have been discussed in particular in connection with closest packings (*e.g.* Cl in NaCl, O in Li_2O, S in ZnS, O in olivine), but numerous examples for non-closest packings are known in addition (*e.g.* B in CaB_6 with $k = 5$; O in rutile with $k = 11$, type 8 in Table 9.1.1.2; Si in α-ThSi$_2$ with $k = 3$). Sphere packings and their voids form the basis for Hellner's framework concept (*cf. e.g.* Hellner *et al.*, 1981). Voids may be calculated systematically as vertices of Dirichlet domains (*cf.* Hellner *et al.*, 1981; Koch, 1984). The tendency to form regular voids of the appropriate size for the cations may counteract the tendency to form an ideal sphere packing of the anions. Examples are spinel and garnet (*cf.* Hellner, Gerlich, Koch & Fischer, 1979).

(3) Frequently, the cations within a crystal structure are also distributed according to a sphere packing. This is explicable because the repulsion between the cations also favours an arrangement with equal but maximal shortest distances (*cf.* Brunner, 1971). In this sense, many crystal structures may be
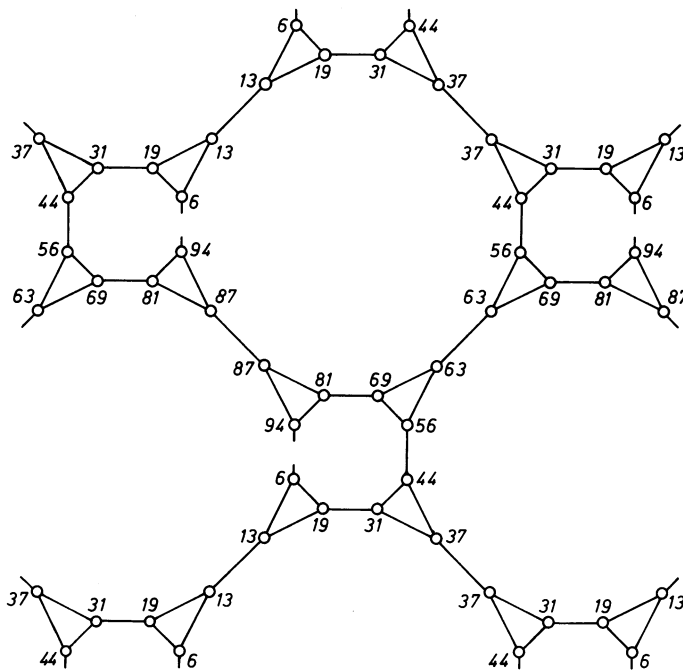

Fig. 9.1.1.6. Sphere packing of type 19 (Table 9.1.1.2) represented by a graph: $k = 10$, $I4/m$, $8(h)$, $xy0$.

Fig. 9.1.1.7. Least dense sphere packing known so far (type 24 of Table 9.1.1.2) represented by a graph: $k = 3$, $I4_132$, $24(h)$, $\frac{1}{8}, y, \frac{1}{4} - y$. z coordinates given in multiples of 1/100.

described as sets of several sphere packings (one for each kind of atom) that are fitted into each other (*e.g.* NaCl, CaF_2, CaB_6, α-$ThSi_2$, rutile, Cu_2O, $CaTiO_3$).

Because of their importance for problems in digital communication (error-correcting codes) and in number theory (solving of diophantine equations), densest sphere packings in higher dimensions are of mathematical interest (*cf.* Conway & Sloane, 1988).

9.1.1.5. *Interpenetrating sphere packings*

Special homogeneous or heterogeneous sets of spheres may be subdivided into a small number i of subsets such that each subset, regarded by itself, forms a sphere packing and that spheres of different subsets do not have mutual contact. Sets of spheres with these properties are called *interpenetrating sphere packings*.

The cubic Laves phases are a well known example for heterogeneous interpenetrating sphere packings. The Mg atoms in $MgCu_2$ [$Fd\bar{3}m$, 8(*a*)], for example, correspond to a sphere packing with shortest distances $d_1 = \sqrt{3}a/4$ and contact number $k = 4$ whereas the copper atoms [16(*d*)] refer to another sphere packing with shortest distances $d_2 = \sqrt{2}a/4$ and $k = 6$. The shortest distances between centres of different spheres are $d_3 = \sqrt{11}a/8 > (d_1 + d_2)/2$.

The crystal structure of Cu_2O gives an example of a different kind. If one takes into account the size of the atoms, sphere contacts can only be expected between different spheres. As a consequence, the heterogeneous set of spheres disintegrates into two heterogeneous but congruent subsets with no mutual contact.

In the case of homogeneous interpenetrating sphere packings, all i subsets have to be symmetry-equivalent. Then the symmetry of each subset is a subgroup of index i of the original space group. Homogeneous interpenetrating sphere packings with cubic symmetry have been derived completely by Fischer & Koch (1976). They may be classified into 39 types. For 33 of the 39 types, the number i of subsets is 2; i is 3, 4, and 8 for 1, 3, and 2 types, respectively.

Remarkable are those homogeneous interpenetrating sphere packings that are built up from sphere packings of type 24 (Table 9.1.1.2), *i.e.* that type with the least dense sphere packing. Combinations of 2, 4, or 8 such sphere packings result in altogether 8 different types of interpenetrating sphere packings (Fischer, 1976). The P atoms in the crystal structure of Th_3P_4 give an example for such interpenetrating sphere packings built up from two congruent subsets (Koch, 1984).

Complete results for other crystal systems are not available. With tetragonal symmetry, interpenetrating sphere packings are known, built up from 2, 3, or 5 congruent subsets (Fischer, 1970). Analogous interpenetration patterns are formed by hydrogen bonds within certain molecular structures (Ermer, 1988; Ermer & Eling, 1988).

Interpenetrating sphere packings may be brought in relation to interpenetrating labyrinths as formed by periodic minimal surfaces or by periodic zero-potential surfaces without self-intersection (*cf. e.g.* Andersson, Hyde & von Schnering, 1984; Fischer & Koch, 1987, 1996; von Schnering & Nesper, 1987).

9.1.2. Packings of ellipses and ellipsoids

The problem of deriving packings of ellipses in two-dimensional space or of ellipsoids in three-dimensional space may be regarded as a generalization of the problem of deriving circle packings and sphere packings. It is much more complicated, however, because a circle or sphere is fully determined by its centre and its radius, whereas the knowledge of the centre, the lengths of the two semiaxes, and the direction of one of them is needed to construct an ellipse. For an ellipsoid, the knowledge of its centre, the length of its three semiaxes, and the directions of two of them is necessary. Accordingly, the point configuration corresponding to the ellipsoid centres does not define the ellipsoid packing and not even its type.

Nowacki (1948) derived 54 homogeneous 'essentially different packings of ellipses'. In contrast to the definition of types of sphere (circle) packings (Section 9.1.1), Nowacki distinguished between similar packings with different plane-group symmetry, *i.e.* between packings that may differ in the orientation of their ellipses. Under an equivalent classification, Grünbaum & Shephard (1987) derived 57 different cases of ellipse packings, thus correcting and completing Nowacki's list. Each of these 57 cases corresponds uniquely to one of the 11 types of circle packings if one takes into account only the contact relations between ellipses and circles. In eight cases, each ellipse has six contacts. Two of these cases can be derived from the densest packing of circles by affine transformations and, therefore, have the same density, namely $\rho = 0.9069$, irrespective of the shape of the ellipses (Matsumoto & Nowacki, 1966). Presumably for the other six cases this density can only be reached (but not exceeded) if the ellipses become circles. A corresponding proof is in progress (Matsumoto, 1968; Tanemura & Matsumoto, 1992; Matsumoto & Tanemura, 1995).

Very little systematic work seems to be carried out on homogeneous or heterogeneous packings of ellipsoids. Matsumoto & Nowacki (1966) derived packings of ellipsoids with contact numbers 12 and high densities by affine deformation of cubic and hexagonal closest packings of spheres. They postulate (without proof) the following: Densest packings of ellipsoids have the same contact number and density as closest packings of spheres and can be derived always from closest sphere packings by affine transformations. If this assumption is true, densest packings of ellipsoids would necessarily consist of parallel ellipsoids only.

Packings of ellipsoids seemed to be useful for the interpretation of the arrangements of organic molecules in crystals. The studies of Kitaigorodsky (1946, 1961, 1973), however, showed that molecular crystals may rather be regarded as dense packings of molecules with irregular shape.

Heterogeneous packings of ellipsoids may possibly be adequate for the geometrical interpretation of some intermetallic compounds like cubic $MgCu_2$ (*cf.* Subsection 9.1.1.4) or Cr_3Si. The ellipsoids enable the use of different 'atomic radii' with respect to neighbouring atoms of the same kind or of different kinds. In $MgCu_2$, for example, the magnesium atoms have cubic site symmetry $\bar{4}3m$ [$Fd\bar{3}m$, 8(*a*)] and therefore can only be represented by spheres. The Cu atoms [16(*d*)] with site symmetry $.\bar{3}m$, however, may be represented by flattened ellipsoids of revolution.

reciprocal space (V^* identified with V) is one with the first m basis vectors lying in V ($m =$ dimension of V).

[v]   *Conventional basis*. For a lattice Λ in three dimensions, it is a basis such that (i) the lattice generated by it is contained in Λ as a sublattice and (ii) there is the standard relationship between the basis vectors (*e.g.* for a cubic lattice a conventional basis consists of three mutually perpendicular vectors of equal length).

The lattice Λ is obtained from the lattice spanned by the conventional basis by adding (a small number of) *centring vectors*. [For example, the b.c.c. lattice is obtained from the conventional cubic lattice by centring the unit cell with $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$.] The reciprocal basis for the conventional basis is a conventional basis for the reciprocal lattice Λ^*.

In the $(m + d)$-dimensional superspace, a conventional basis for the lattice Σ satisfies the same conditions (i) and (ii) as formulated above for the three-dimensional case. In addition, however, one requires that the basis is standard and such that the non-vanishing external components satisfy the relations of an ($m = 3$) conventional basis and that the corresponding internal components only involve the irrational components of the modulation vector(s) (for $d = 1$ the basis is such that $\mathbf{q}^r = 0$, thus $\mathbf{q}^i = \mathbf{q}$). Again a conventional basis for Σ^* is dual to the same for Σ.

[vi]   *Holohedry*. The holohedry of a vector module is the group of orthogonal transformations of the same dimension that leaves the vector module invariant. The holohedry of an $(m + d)$-dimensional lattice is the subgroup of $O(m) \times O(d)$ that leaves the lattice invariant.

[vii]   *Point group*. An $(m + d)$-dimensional crystallograhic point group $K_s = (K_E, K_I)$ is a subgroup of $O(m) \times O(d)$. With respect to a standard lattice basis its elements $R_s = (R, R_I)$ are of the form

$$\Gamma(R) = \begin{pmatrix} \Gamma_E(R) & 0 \\ \Gamma_M(R) & \Gamma_I(R) \end{pmatrix},$$

where all the entries are integers and R is an element of an m-dimensional point group K, which is actually the same as K_E. For an incommensurate modulated crystal, K_s and K are isomorphic groups. If $d = 1$, $\Gamma_I(R) = \varepsilon = \pm 1$.

[viii]   *Geometric crystal class*. Two point groups $K_s = (K_E, K_I)$ and $K'_s = (K'_E, K'_I)$ of pairs (R_E, R_I) of orthogonal transformations [R_E belongs to $O(m)$ and R_I to $O(d)$] are geometrically equivalent if and only if there are orthogonal transformations T_E and T_I of $O(m)$ and $O(d)$, respectively, such that $R'_E = T_E \cdot R_E \cdot T_E^{-1}$ and $R'_I = T_I \cdot R_I \cdot T_I^{-1}$ for some group isomorphism $(R_E, R_I) \rightarrow (R'_E, R'_I)$. For $d = 1$, that condition takes a simpler form because $R_I = \varepsilon = \pm 1$.

[ix]   *Arithmetic crystal class*. A group of integral matrices $\Gamma^*(R)$ [for $R \in K$ of $O(m)$] is determined on a basis $\{\mathbf{a}_i^*; i = 1, \ldots, n\} = \mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*, \mathbf{q}_1, \ldots, \mathbf{q}_d$ of a vector module in reciprocal space by an m-dimensional point group K (here $m = 3$). For modulated crystals, the transformations in direct space are given by matrices $\Gamma(R) =$ transpose of $\Gamma^*(R^{-1})$ which are of the form (9.8.4.17). Two groups $\Gamma'(K')$ and $\Gamma(K)$ are arithmetically equivalent if and only if there is an $(m + d)$-dimensional matrix S of the form

$$S = \begin{pmatrix} S_E & 0 \\ S_M & S_I \end{pmatrix}$$

with integral entries and determinant ± 1 such that $\Gamma'(K') = S\Gamma(K) \cdot S^{-1}$. Here S_E is $m \times m$ and S_I is $d \times d$ dimensional. An alternative formulation is: the matrix groups $\Gamma(K)$ and $\Gamma'(K')$ determined as in equation (9.8.1.16) or in equation (9.8.1.21) are arithmetically equivalent if

(*a*) the groups K and K' are geometrically equivalent m-dimensional point groups [the corresponding $(m + d)$-dimensional point groups K_s and K'_s are then also geometrically equivalent];

(*b*) there are vector module bases $\mathbf{a}^*, \ldots, \mathbf{q}_d$ and $\mathbf{a}^{*\prime}, \ldots, \mathbf{q}'_d$ such that K on the first basis gives the same group of matrices as K' on the second basis.

[x]   *Bravais class*. Two vector modules are in the same Bravais class if the groups of matrices determined by their holohedries are arithmetically equivalent. Two $(m + d)$-dimensional lattices are in the same Bravais class if their holohedries are arithmetically equivalent. In both cases, one can find bases for the two structures such that the holohedries take the same matrix form. In the $(m + d)$-dimensional case, the lattice bases both have to be standard.

[xi]   *Superspace group*. An $(m + d)$-dimensional superspace group is an n-dimensional space group ($n = m + d$) such that it has a d-dimensional lattice of internal translations. (This latter property reflects the periodicity of the modulation.) It is determined on a standard lattice basis by the matrices $\Gamma(R)$ of the point-group transformations and by the components $\upsilon_i(R)$ ($i = 1, \ldots, m + d$) of the translation parts of its elements. The matrices $\Gamma(R)$ represent at the same time the elements R of the m-dimensional point group K and the corresponding elements R_s of the $(n + d)$-dimensional point groups K_s. Two $(m + d)$-dimensional superspace groups are equivalent if there is an origin and a standard lattice basis for each group such that the collection $\{\Gamma(K), \upsilon_s(K)\}$ is the same for both groups. [In previous formulae, $\upsilon_s(R)$ is often simply indicated as υ_s.]

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