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, 3^46, 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 *p*6*mm* 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, 1991*a*,*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 $k = 4$.