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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.

references